THE SPECTRUM OF THORIUM FROM 250 nm TO 5500 nm: RITZ WAVELENGTHS AND OPTIMIZED ENERGY LEVELS

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Received 2013 April 18; accepted 2013 August 22; published 2014 February 6

ABSTRACT

We have made precise observations of a thorium–argon hollow cathode lamp emission spectrum in the region between 350 nm and 1175 nm using a high-resolution Fourier transform spectrometer. Our measurements are combined with results from seven previously published thorium line lists to re-optimize the energy levels of neutral, singly, and doubly ionized thorium (Th I, Th II, and Th III). Using the optimized level values, we calculate accurate Ritz wavelengths for 19,874 thorium lines between 250 nm and 5500 nm (40,000 cm$^{-1}$ to 1800 cm$^{-1}$). We have also found 102 new thorium energy levels. A systematic analysis of previous measurements in light of our new results allows us to identify and propose corrections for systematic errors in Palmer & Engleman and typographical errors and incorrect classifications in Kerber et al. We also found a large scatter with respect to the thorium line list of Lovis & Pepe. We anticipate that our Ritz wavelengths will lead to improved measurement accuracy for current and future spectrographs that make use of thorium–argon or thorium–neon lamps as calibration standards.

Key words: atomic data – line: identification – methods: data analysis – standards – techniques: radial velocities

Online-only material: machine-readable tables

1. INTRODUCTION

Fifty years ago the spectrum of thorium was studied in several laboratories as a source of wavelength standards for high-resolution grating spectrographs, resulting ultimately in an extensive list of proposed secondary standards (Giacchetti et al. 1970). More recently, measurements with very high precision and internal consistency were published by Palmer & Engleman (1983, hereafter PE83). These measurements were made on the 1 m Fourier transform spectrometer (FTS) of the National Solar Observatory at Kitt Peak (Braut 1976) using a commercial thorium–neon hollow-cathode lamp (HCL) run at the unusually high current of 75 mA. The lamp was observed in five overlapping spectral regions covering 277.7 nm through 1350.0 nm (7400 cm$^{-1}$ through 36,000 cm$^{-1}$). PE83 estimated their uncertainties ($\delta_{\sigma,\text{PE83}}$) in units of 0.001 cm$^{-1}$ based upon an empirical fit to the equation

$$\delta_{\sigma,\text{PE83}}[10^{-3} \text{ cm}^{-1}] = \frac{a}{\lambda} + b\sigma,$$

where $\lambda$ is the intensity of the line, $\sigma$ is its wavenumber (\text{cm}^{-1}) = $10^{4}/\lambda$(nm), and $a$ and $b$ are coefficients, which they determined to be 0.5 and $5 \times 10^{-5}$, respectively (note that PE83 incorrectly reported the coefficient $b$ as $0.5 \times 10^{-5}$). The first term in this empirical formula is the statistical uncertainty of the measurement of the line, and the second is the systematic uncertainty attributable to the global calibration of the spectra.

The thorium spectrum has been measured several more times since 1983. Most notably, it was measured in the near-ultraviolet (NUV) and visible regions by Lovis & Pepe (2007, hereafter LP07) using the High-Accuracy Radial-velocity Planet Searcher (HARPS; Pepe et al. 2000). LP07 used the PE83 wavelength measurements to determine the dispersion solution for HARPS and measure faint thorium lines that did not appear in PE83. They also reported reduced uncertainties for many of the thorium lines observed in PE83. The thorium spectrum was also measured in the near-infrared (NIR) through 5500 nm (1800 cm$^{-1}$) at a lamp current of 320 mA by Engleman et al. (2003, hereafter EHW03) using the McMath 1 m FTS. Finally, the NIR spectrum was measured with the National Institute of Standards and Technology (NIST) 2 m FTS (Nave et al. 1997) from 691 nm to 5804 nm with a hollow cathode lamp running at 20 mA by Kerber et al. (2008, hereafter KNS08). Also since 1983, a number of thorium lines have been measured with high accuracy by laser spectroscopy (Sansonetti & Weber 1984; DeGraffenreid & Sansonetti 2002; DeGraffenreid et al. 2012, collectively referred to hereafter as LS3). These lines can be used to recalibrate the results of PE83, reducing the systematic contribution to their uncertainties.

Thorium–argon (Th/Ar) HCLs are installed on many of the highest-precision astronomical spectrographs, including the European Southern Observatory’s (ESO’s) Cryogenic high-resolution InfraRed Echelle Spectrograph (CRIRES; Käufl et al. 2004), the High-Resolution Spectrograph (HRS; Tull 1998) on the Hobby-Eberly Telescope (HET; Ramsey et al. 1998), and HARPS. HARPS is currently the most precise astronomical spectrograph in the world, and typically achieves radial velocity precision below 1 m s$^{-1}$ (a relative precision of 3 parts in $10^6$; Mayor et al. 2009).

Exoplanet radial velocity measurements, such as those made with the HARPS spectrograph, attempt to detect periodic variations in stellar wavelengths; therefore, they do not usually depend upon the absolute accuracy of the calibration source as long as the calibration lines are precisely reproducible. However, systematic errors in the spectrograph can increase the uncertainty of the measured radial velocities. An example of such systematic errors can be seen in Figure 4 of Wilken et al. (2010), where the authors show the difference between the dispersion solutions found using a Th/Ar lamp and a laser frequency comb across the same order of the HARPS spectrograph. Since the LP07 line list was based on observations with the HARPS spectrograph, such errors in the dispersion solution undoubtedly affect their thorium wavelengths.

In an effort to provide the physics and astrophysics communities with thorium wavelengths of higher accuracy, we have re-measured more than 1600 thorium lines in the NUV to NIR.
Additionally, we have performed least-squares energy level optimizations for Th\textsubscript{I}, Th\textsubscript{II}, and Th\textsubscript{III} using classified lines from our measurements and previous work. The optimization provides precise level values from which we calculate Ritz wavelengths for all observed lines of thorium that we can classify throughout the optical and near-infrared. Since these Ritz wavelengths are calculated from globally optimized energy levels, they are usually more precise than the measured wavelengths.

In Section 2, we lay out the motivation for this paper. In Section 3, we describe our new measurements and compare them to previously reported line lists. In Section 4, we describe how we adjusted and used data from various sources to classify thorium lines throughout the optical and near-infrared; re-optimized the levels of neutral, singly, and doubly ionized thorium; and calculated Ritz wavelengths. This section includes an abbreviated list. Finally, in Section 5, we summarize the work and draw some conclusions.

2. MOTIVATION FOR AN UPDATED LINE LIST

Atomic emission lines are caused by transitions of electrons from an upper energy level to a lower energy level. Atomic energy levels are usually not measured directly, but can be inferred by searching large numbers of emission or absorption lines for common differences between unclassified lines and known energy levels. If the energies of the combining levels are accurately known, the wavenumber and corresponding wavelength of the transition can be calculated by simply differencing the energies. These calculated values are known as Ritz wavelengths and are often more accurate than experimental measurements due to the large number of measured transitions that determine each energy level.

In the case of thorium, a large number of energy levels of Th\textsubscript{I} and Th\textsubscript{II} were accurately determined in the work of PE83. Ritz wavelengths based on these energy levels can be used to classify observed lines in newly acquired thorium spectra. Observed spectral lines that do not match Ritz wavelengths within their expected uncertainties fall into several categories. Assuming that the spectrograph itself is not responsible for introducing systematic errors, either (1) the spectral line is formed by a transition between two energy levels one or both of which is not known, (2) one or both energy level values is inaccurate, (3) the observed spectral line is attributable to some other element contaminating the source, or (4) the observed line is shifted by a blend with another line, which is not resolved in the spectrum.

This work was undertaken in an attempt to determine whether some of the many unidentified lines in the LP07 line list could be classified by comparing their measured wavelengths to thorium Ritz wavelengths. We hoped that this comparison would provide two distinct benefits. First, it would help us determine which unidentified lines in the LP07 line list are thorium lines that can be used for precise wavelength calibration and which ones are calculated from globally optimized energy levels, they are usually more precise than the measured wavelengths.

PE83 wavelengths (dotted histogram). There are two possible explanations for this observation. First, it is possible that the energy levels of Th\textsubscript{I} and Th\textsubscript{II} as presented in PE83 need to be updated. A re-optimization of the energy levels using the wavenumbers of LP07 might provide a more accurate and internally consistent set of energies than those reported by PE83.

The second possibility is that the LP07 wavelengths are less accurate than the PE83 wavelengths. This would be surprising since one of the primary motivations behind the LP07 line list

\begin{figure}[ht]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Distribution in differences between the measured wavelengths and closest Ritz wavelengths of four populations of thorium wavelength measurements. All Ritz wavelengths were calculated using energy levels published in the online actinides database (web2.lac.u-psud.fr/lac/Database/Tab-energy/Thorium/Th-el-dir.html). The thorium lines of Palmer & Engleman (1983) are shown as a dash–dotted line, the unidentified emission lines of Lovis & Pepe (2007) are shown as a solid line, and the PE83 thorium lines as measured by LP07 are shown as a dotted line. A set of uniformly distributed random wavelengths are shown with the dashed histogram. The thorium lines of PE83 show the best agreement with the Ritz wavelengths.

\begin{itemize}
\item actinide energy levels,\footnote{http://web2.lac.u-psud.fr/lac/Database/Tab-energy/Thorium/Th-el-dir.html} with uncertainties of 0.001 cm\(^{-1}\) for Th\textsubscript{I} and Th\textsubscript{II} levels. For clarity, the distributions have been truncated below 5 \(\times\) 10\(^{-6}\). A single histogram bar below this value indicates the sum of the distribution tail below this value. The standard deviation of the difference between PE83 and the Ritz wavelengths is 8.2 \(\times\) 10\(^{-5}\) nm, while the corresponding quantity for LP07 is 13.2 \(\times\) 10\(^{-5}\) nm. The black histogram (solid line) is the corresponding distribution for the many unidentified emission lines reported by LP07. This histogram is double-peaked, probably due to the presence of both (1) thorium lines that match their Ritz wavelengths to within about 0.001 nm (lower-difference peak) and (2) argon lines, unknown lines, and thorium transitions between unknown energy levels (higher-deviation peak). This latter peak is similar to the distribution found when random wavelengths are compared to the 21,440 theoretically possible thorium Ritz wavelengths between 370 and 700 nm (14,000 cm\(^{-1}\) and 27,000 cm\(^{-1}\)) as illustrated by the dashed line in Figure 1.
\end{itemize}

It is clear that the LP07 lines do not agree with the Ritz wavelengths as well as the same lines observed by PE83. This is to be expected, since many of the energy levels come from the PE83 data. However, the disagreement between the unidentified LP07 lines and the closest Ritz wavelengths (solid histogram) is surprisingly large. Surely many of these lines must involve transitions between known thorium energy levels, but the distribution does not resemble the LP07 measurements of PE83 wavelengths (dotted histogram). There are two possible explanations for this observation. First, it is possible that the energy levels of Th\textsubscript{I} and Th\textsubscript{II} as presented in PE83 need to be updated. A re-optimization of the energy levels using the wavenumbers of LP07 might provide a more accurate and internally consistent set of energies than those reported by PE83.

The second possibility is that the LP07 wavelengths are less accurate than the PE83 wavelengths. This would be surprising since one of the primary motivations behind the LP07 line list...}
was to provide lower uncertainties than PE83. Their uncertainties, calculated by using Equation (1), are typically between 2 × 10^−5 nm and 10 × 10^−3 nm (15 m s^−1 to 62 m s^−1). By comparison, the LP07 uncertainties for the same lines (as published) are between 1 × 10^−5 nm and 76 × 10^−5 nm (7 m s^−1 to 600 m s^−1), with several thousand lines having uncertainties substantially reduced with respect to PE83.

In an attempt to understand the discrepancies between the results of PE83 and LP07, we recorded a new thorium spectrum with the 2 m FTS at NIST. There are several advantages to using an FTS (as opposed to an echelle spectrograph) to measure wavelengths in emission spectra. First and foremost, the dispersion solution of an FTS is linear in wavenumber. As long as a few standard lines, measured independently to high accuracy, are in the observed spectrum, the entire dispersion solution can be calibrated to a similar accuracy. Second, the signal-to-noise ratio (S/N) in the spectrum can be improved by increasing the integration time without fear of saturating even the brightest emission lines. Third, the very high resolving power of the FTS (as high as 10^7 in the case of the NIST 2 m FTS) means that blended lines are less common and that noble gas lines can often be distinguished from heavier elements on the basis of their measured widths alone. Finally, the high resolution of the FTS means that uncertainties in determining the positions of individual lines are much smaller than can be achieved with lower-resolution instruments (see Equation (6)).

3. NEW MEASUREMENTS OF THORIUM

3.1. Experimental Setup

We observed the spectrum of a commercial sealed Th/Ar HCL running at 25 mA for almost 15 hr starting on 2011 November 2. The spectrum was recorded between 0 cm^−1 and 30,000 cm^−1 at a sampling resolution of 0.02 cm^−1. The region of observation was limited to between 8500 cm^−1 and 28,000 cm^−1 (360 nm and 1200 nm) by the sensitivity of the silicon photodiode detector. The FTS enclosure was evacuated to a pressure of about 2 × 10^−5 Pa (0.0197 Torr) throughout the observation. Low resolution spectra of a radiometrically calibrated tungsten ribbon lamp were recorded before and after the thorium spectrum so that we could determine the spectral response of the FTS. The response function derived from these spectra was used to obtain radiometrically calibrated relative intensities for the emission lines from the HCL.

Our new spectrum was calibrated with respect to thorium lines precisely measured by LS3. It provides a direct comparison to the results of PE83 in that it spans portions of all five of their thorium–neon spectra. Because Palmer & Engleman did not have good internal standards across the entire spectrum, they arbitrarily chose to take as their calibration factor the finite aperture correction for the 11,000 cm^−1 to 18,000 cm^−1 (550 nm to 900 nm) spectral region. This calibration was propagated to the other four spectral regions by using overlapping lines. No internal standard lines were used for calibration. Thus it is very valuable to have a comparison spectrum with a well-defined calibration that overlaps with all of the PE83 regions.

3.2. Measurements and Uncertainties

The spectrum was measured by fitting a Voigt function to each emission line with an S/N of greater than 20 using the program XGremlin (Nave et al. 1997), an X-windows implementation of GREMLIN (Brault & Abrams 1989). The spectrum was interpolated by convolution with the FTS instrumental function before fitting the Voigt profile. The initial wavenumber scale was based on the optical path difference measured by the helium–neon control laser of the FTS as the interferogram was recorded. However, even in the case of perfect alignment, the optical path difference for an emission source is slightly different from that measured by the control laser because of the finite instrumental aperture. This results in a stretching of the wavenumber scale which we correct in the usual way by determining a multiplicative correction factor κi from internal standard lines:

\[
κ_i = \frac{σ_{\text{std},i}}{σ_{\text{obs},i}} - 1,
\]

where σ_{\text{std},i} is the accurately known wavenumber of the standard line, and σ_{\text{obs},i} is the uncorrected wavenumber of the same line.

The uncertainty in the individual wavenumber correction factor (δκ,i) is the sum in quadrature of the relative uncertainty in the standard wavenumber and the relative statistical uncertainty of the measured line:

\[
δκ,i = \sqrt{\left(\frac{δσ_{\text{std},i}}{σ_{\text{std},i}}\right)^2 + \left(\frac{δσ_{\text{obs},i}}{σ_{\text{obs},i}}\right)^2},
\]

where δσ_{\text{obs},i} is the statistical uncertainty in the line centroid derived from Equation (9.2) of Davis et al. (2001). Our spectra are under-sampled, so there is only one statistically independent point in a line width:

\[
δκ,i = \frac{W_i}{S/N_i \sqrt{N_{w,i}}},
\]

where W_i is the measured line width at half-maximum, S/N_i is the measured signal-to-noise ratio of the line, and N_{w,i} is the number of significant points in the width of the line, which is equal to the line width divided by the spectral resolution.

The overall correction factor for the spectrum, κ, is taken to be the mean of the individual wavenumber correction factors, weighted by the inverse square of their uncertainties:

\[
κ = \frac{\sum κ_i δκ,i^{-2}}{\sum δκ,i^{-2}}.
\]

All wavenumbers in the spectrum are corrected by multiplying by the factor (1 + κ). The uncertainty (δκ) in κ is taken to be the standard error of the mean of individual κ_i values.

The final uncertainty of each of our measured wavenumbers is the sum in quadrature of the calibration uncertainty and the statistical uncertainty of the line centroid:

\[
δκ,i = \sqrt{δκ,i^2 + δκ,i^2}.
\]

The determination of the wavenumber correction factor for our Th/Ar spectrum is illustrated in Figure 2. We compared values of the correction factor as determined from three atomic species: neutral argon (Ar i), singly ionized argon (Ar ii), and neutral thorium (Th i). The Ar i standards are low-excitation lines from Whaling et al. (2002) with corrections from Sansonetti (2007), while the Ar ii standards are from Whaling et al. (1995). For thorium standards, we used 30 of the 31 lines measured by laser spectroscopy by LS3. One line (at 15,966.4061 cm^−1, 626.315022 nm) was not used because it is suspected to be a blend (Sansonetti & Weber 1984), and
Indeed it was an outlier compared to our newest measurements at NIST. We suspect that this line is a blend of the thorium lines only, as the correction factor for the spectrum.

### 3.3. Results

We measured the wavenumbers of 1644 thorium lines between 350 nm (28,570 cm<sup>-1</sup>) and 1175 nm (8510 cm<sup>-1</sup>). Identifications of lines as thorium were based primarily on their observed line widths. Thorium line widths were typically between 0.03 cm<sup>-1</sup> and 0.04 cm<sup>-1</sup> (1 × 10<sup>−6</sup> nm and 3 × 10<sup>−6</sup> nm), and argon line widths were typically between 0.05 cm<sup>-1</sup> and 0.09 cm<sup>-1</sup> (3 × 10<sup>−6</sup> nm). Thorium lines that could be matched unambiguously to Ritz wavelengths have been classified. A sample of our new measurements is presented in Table 1, which is generally self-explanatory. The rightmost column contains the difference between our measured wavenumber and the Ritz wavenumber calculated from our re-optimized thorium energy levels as discussed below.

### 3.4. Comparison with Previous Thorium Line Lists

We compared our thorium measurements to three previously published line lists: the Th/Ne measurements of PE83, which were made using the Kitt Peak FTS; the Th/Ar measurements of KNS08, which were made using the NIST 2 m FTS; and the Th/Ar measurements of LP07, which were made using the HARPS echelle spectrograph. The Th/Ar spectrum of EHW03 includes lines between 1798 cm<sup>-1</sup> and 9180 cm<sup>-1</sup> (1089 nm to 5562 nm), mostly outside of our observed range. The line list of EHW03 is in good agreement with the measurements of KNS08 in their region of overlap.

It is not uncommon for papers in the scientific literature to report general uncertainties, rather than uncertainties for individual lines. The relative contribution of systematic and random factors to these general uncertainties is often ill defined. In such cases, it is difficult or impossible to assign appropriate uncertainties to the wavelengths if the data are recalibrated using improved standards that reveal previously unknown systematic errors. We have estimated the statistical uncertainties of previously reported measurements by comparing the measured wavenumbers to the Ritz wavenumbers (after optimizing the energy levels; see Section 4). This process conflates the statistical uncertainties with any systematic uncertainties, so in these cases, we added the statistical and systematic uncertainties.
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Figure 3. Wavenumber correction factor $\kappa$ determined for the Th/Ne line list of PE83, using their published wavenumbers and wavenumber uncertainties. This wavenumber correction factor is in addition to the wavenumber correction factor of $5.05838 \times 10^{-7}$ applied to the PE83 spectrum by its authors.

Figure 4. Comparison between our measured wavenumbers and three historical sources, all shown on the same scale: PE83 (top), KNS08 (middle), and LP07 (bottom). These plots only compare lines for which our uncertainty was less than $0.0004 \text{ cm}^{-1}$ and the signal-to-noise ratio of our lines was greater than 100 (about 10% of the lines). The error bars are the sum in quadrature of our NIST measurements and the uncertainties of PE83, LP07, or KNS08, respectively. The mean and standard deviation of each difference is printed in the upper left corner of each plot. The PE83 measurements have been corrected by a $\kappa$ of $2.2 \times 10^{-8}$ (see Figure 3). The PE83 uncertainties are the published uncertainties (using Equation (1)). Hash marks in the lower part of this panel indicate the overlap between different spectra in PE83.

The difference between our new thorium measurements (hereafter, RNS13) and the re-calibrated results of PE83—shown in the top panel of Figure 4—reveal some minor systematic trends in the data of PE83. First, there are at least two places in the spectrum where the differences systematically rise and fall. These can be seen at about 12,000 cm$^{-1}$ and 18,000 cm$^{-1}$ (830 nm and 550 nm, respectively). The feature at 18,000 cm$^{-1}$ corresponds to a region where measurements from overlapping spectra were combined, but the feature

linearly. We found that the best fit for the statistical uncertainties could be represented by functions of the form:

$$\delta\sigma,i = \delta_\kappa \sigma_i + c / I_i^d,$$

(7)

where $c$ and $d$ are coefficients, and $I_i$ is the reported intensity of the line. This function is similar to the equation used by PE83 to estimate their statistical uncertainties (see Equation (1)).

3.4.1. Comparison with Palmer & Engleman (1983)

The measurements of PE83 were made by combining results from five overlapping spectra from the Kitt Peak FTS. Until the introduction of LP07, this line list was widely used throughout the astrophysical community to calibrate Th/Ar spectra.

In 1983, Palmer & Engleman had no internal standards known with sufficient accuracy to determine their wavenumber correction factor. Since then, the wavenumbers of several thorium lines have been measured via laser spectroscopy by Sansonetti & Weber (1984; fifteen lines), DeGraffenreid & Sansonetti (2002; seven lines), and DeGraffenreid et al. (2012; eight lines). Saloman & Sansonetti (2004) also compiled thousands of neon lines, some of which are recommended as standards. Using the thorium and neon wavenumber measurements of PE83, we have redetermined the wavenumber correction factor of the PE83 line list (Figure 3). In light of the trend and large scatter in the neon results, we have used the thorium lines to calculate a revised wavenumber correction factor for the results of PE83. Note that a similar trend in the neon standards was seen in Redman et al. (2011).

The PE83 line list is a compilation of several, independently measured spectra. It is unlikely that they all share the same uncertainty relationship. Therefore, we have estimated the uncertainties of PE83 in each of the spectral regions by fitting the standard deviation of the differences between the measured wavenumber and the Ritz wavenumbers as a function of intensity. The uncertainties are then given by Equation (7). The $c$ and $d$ coefficients are different for the different spectral regions of the line list (which was segmented at—roughly—11,000 cm$^{-1}$, 18,000 cm$^{-1}$, 21,000 cm$^{-1}$, 25,000 cm$^{-1}$, 30,000 cm$^{-1}$, or 900 nm, 550 nm, 480 nm, 400 nm, and 330 nm), and are summarized in Table 2. We set the calibration uncertainty throughout to be $1.2 \times 10^{-8} \times \sigma_{PE83}$.

![Table 2](https://example.com/table2.png)

| Spectral Range | $c$ (cm$^{-1}$) | $d$ (cm$^{-1}$) |
|---------------|----------------|----------------|
| <11000        | 0.00053        | 0.678          |
| 11000–18000   | 0.00192        | 0.482          |
| 18000–21000   | 0.00165        | 0.462          |
| 21000–25000   | 0.00171        | 0.404          |
| 25000–30000   | 0.00331        | 0.405          |
| >30000        | 0.00324        | 0.531          |

The difference between our new thorium measurements (hereafter, RNS13) and the re-calibrated results of PE83—shown in the top panel of Figure 4—reveal some minor systematic trends in the data of PE83. First, there are at least two places in the spectrum where the differences systematically rise and fall. These can be seen at about 12,000 cm$^{-1}$ and 18,000 cm$^{-1}$ (830 nm and 550 nm, respectively). The feature at 18,000 cm$^{-1}$ corresponds to a region where measurements from overlapping spectra were combined, but the feature
at 12,000 cm\(^{-1}\) is not at a boundary point between two spectra. The latter feature corresponds to a local minimum in the reflectivity of aluminum, so we speculate that PE83 used a low-resolution transform when determining the phase. Second, the PE83 wavenumbers are systematically smaller than ours below 11,000 cm\(^{-1}\) (900 nm) and above about 20,000 cm\(^{-1}\) (500 nm). The trend above 20,000 cm\(^{-1}\) corresponds to the linear trend in the wavenumber correction factor of PE83 shown in Figure 3. Since we see this same deviation when we compare the PE83 wavenumber measurements to the laser-spectroscopy measurements of DeGraffenreid et al. (2012), but not when we compare our own measurements to these standards, this suggests the trend exists in the PE83 line list.

3.4.2. Comparison with Kerber et al. (2008)

The near-infrared Th/Ar line list of Kerber et al. (2008) was based on observations with the 2 m FTS at NIST, the same spectrometer we used to make our measurements. It should be noted that we are using a different beam splitter, mirrors, and detector, and we would not expect any systematics to be common between the observations. Our measurements are in agreement with Kerber et al. (2008) to within 1 part in 10\(^8\). We see no systematic bump in the KNS08 line list measurements around 12,000 cm\(^{-1}\) (830 nm)—indeed, KNS08 also saw a systematic deviation from the wavenumbers of PE83 (see their Figure 7). This is further evidence that this deviation represents a local systematic error in the line list of PE83.

3.4.3. Comparison with Lovis & Pepe (2007)

Lovis & Pepe (2007) measured the wavelengths of thorium lines between about 380 nm and 690 nm (26,000 cm\(^{-1}\) and 14,500 cm\(^{-1}\), respectively) using the echelle spectrograph HARPS. Because of the high sensitivity of their echelle spectrograph, they saw thousands of lines not reported by PE83. The primary motivations of their work were to provide more accurate thorium wavelengths than those published in PE83 and to measure the wavelengths of unknown emission lines that were observable in the HARPS spectra. However, the comparison between our thorium measurements and those of LP07 shows a large scatter, seen in the bottom panel of Figure 4, that is about 2.5 times larger than the average uncertainty. This is in sharp contrast to our agreement with the PE83 thorium line measurements—top panel of Figure 4), and suggests that the LP07 uncertainties were underestimated.

This large scatter probably comes from a number of sources, including systematic offsets in the HARPS detectors (such as the imperfect stitching of the multiple detectors in the spectrograph focal plane found by Wilken et al. 2010) and shifts due to unresolved blending of adjacent lines. LP07 assumed (incorrectly) that their measurements were much more precise than those of PE83 because of the high S/N of their spectra. As a consequence, they attributed any differences between their measurements and those of PE83 to systematic errors or random noise in the measurements of the latter. Our analysis suggests that the discrepancies actually come largely from systematic errors in the measurements of LP07.\(^2\)

Given that their uncertainties were underestimated, we wondered if some of the lines not identified in LP07 might actually have been measured in PE83. The distribution of absolute differences between the unidentified LP07 lines (classified as “?” in their line list) and the closest PE83 lines is shown in Figure 5. There is a clear population bump of lines with differences less than about 0.05 cm\(^{-1}\). To investigate these lines we plotted a HARPS Th/Ar spectrum and one of the PE83 Th/Ne spectra on the same scale, and found that 231 of the “?” lines of LP07 were clearly coincident within 0.05 cm\(^{-1}\) with lines in the spectra of PE83 as illustrated in Figure 6. Most of these lines are perturbed by blending with nearby lines in the lower resolution HARPS spectra. Figure 7 shows the differences between these LP07 lines and the measurements of the same lines by PE83. The uncertainties shown are the sum in quadrature of the published uncertainties. The ratio between the size of the deviation

\(^2\) It is worth noting that grating spectrometers have much higher efficiencies than Fourier transform spectrometers, and represent one of the few ways to find and measure the fainter thorium lines. It should be possible to use grating spectrographs to measure these fainter thorium lines, but it is essential that the FTS-measured thorium lines be treated as standards throughout the process. The more accurate FTS measurements should be used to estimate (and possibly correct) the systematic errors of the grating spectograph dispersion solutions before estimating the wavelengths and uncertainties of the unknown lines.
and the published uncertainty is as large as 25, suggesting that for blended lines the LP07 uncertainties may be underestimated by more than an order of magnitude.

Many additional lines are seen in the HARPS spectra that are not in the spectra of PE83. Among these lines are weak thorium lines, argon lines, lines from trace contamination of other elements, and possibly artifacts from the optics of HARPS. Using calculated Ritz wavelengths, as well as compilations such as the atomic spectra database3 (Ralchenko et al. 2011) and the MIT wavelength tables (Harrison 1969), we have identified over 1700 of these lines, including 1622 thorium lines, 94 argon lines, and a few lines of contaminant elements. Since some argon lines are known to show shifts of as much as 6 \times 10^{-3} \text{ cm}^{-1} (tens of m s^{-1}), depending on the lamp pressure (Whaling et al. 2002; Lovis et al. 2006), these lines should not be used as calibration lines. Likewise, contaminant lines and lines that remain unidentified and may be optical artifacts are not suitable for calibration. Lovis et al. (2006) mentions future plans to help identify thorium lines, but it does not appear that these results were published.

To identify possible contaminant sources, we referred to Tables III and IV of the MIT Wavelength Tables (Harrison 1969). These lists of sensitive lines are compiled from empirical observation, and include lines from the various elements that are most likely to appear in arc and spark discharges when only a small quantity of that element is present. Based on the presence of these sensitive lines in the HARPS Th/Ar spectra, we have identified lines of calcium (Ca), chromium (Cr), magnesium (Mg), and manganese (Mn). PE83 noted contamination from all of these elements except Mn in their spectra.

4. OPTIMIZED ENERGY LEVELS AND RITZ WAVELENGTHS

From our own observations and previously published sources, we have assembled a list of 19,874 classified thorium lines between 250 nm and 5500 nm that were used to re-optimize the previously reported levels of Thi, Thii, and Thiii. Lines were drawn from eight different sources. Five of these sources—PE83, EHW03, LP07, KNS08, and RNS13—have already been discussed. We also incorporated data from three other publications. Giacchetti et al. (1974, hereafter GBCZ74) report FTS observations of 3100 thorium lines (2300 classified) in the region 900 nm to 3000 nm. Zalubas & Corliss (1974, hereafter ZC74) and Zalubas (1976, hereafter Z76) include 6485 classified lines of Thii and 9587 classified lines of Thi, respectively. ZC74 and Z76 are compilations of measurements from a variety of experimental sources.

3 http://www.nist.gov/pml/data/asd.cfm
## Table 4
New Thorium Energy Levels

| Energy (cm⁻¹) | Energy Uncertainty (cm⁻¹) | J | N | Energy (cm⁻¹) | Energy Uncertainty (cm⁻¹) | J | N |
|---------------|---------------------------|---|---|---------------|---------------------------|---|---|
| 32605.50954   | 0.0004                    | 1 | 16| 40697.4116    | 0.0013                    | 2 | 3 |
| 34088.0343    | 0.0005                    | 2 | 21| 40789.3803    | 0.0006                    | 5 | 14|
| 35108.8155    | 0.0006                    | 2 | 18| 41010.1262    | 0.0011                    | 3 | 11|
| 35497.6156    | 0.0009                    | 2 | 12| 41039.8704    | 0.0013                    | 2 | 12|
| 37126.4931    | 0.0009                    | 1 | 5 | 41285.4358    | 0.0015                    | 3 | 16|
| 37472.7204    | 0.0009                    | 1 | 7 | 41500.6175    | 0.0007                    | 3 | 11|
| 38443.8055    | 0.0007                    | 3 | 14| 41548.5831    | 0.0004                    | 6 | 9 |
| 38763.4763    | 0.0005                    | 5 | 13| 41557.8339    | 0.0011                    | 3 | 12|
| 39160.8499    | 0.0006                    | 2 | 13| 41939.3407    | 0.0005                    | 5 | 12|
| 39997.6156    | 0.0012                    | 2 | 12| 41940.6340    | 0.0013                    | 4 | 9 |
| 40024.9810    | 0.0006                    | 3 | 9 | 42096.1941    | 0.0015                    | 3 | 12|
| 40280.9864    | 0.0008                    | 2 | 13| 42774.0660    | 0.0011                    | 6 | 7 |
| 40350.5849    | 0.0012                    | 3 | 12| 42824.6699    | 0.0012                    | 4 | 12|
| 40577.1845    | 0.0004                    | 3 | 17| 42839.5573    | 0.0012                    | 3 | 11|
| 40637.5755    | 0.0006                    | 6 | 11| 42891.6858    | 0.0013                    | 4 | 12|

| Energy (cm⁻¹) | Energy Uncertainty (cm⁻¹) | J | N | Energy (cm⁻¹) | Energy Uncertainty (cm⁻¹) | J | N |
|---------------|---------------------------|---|---|---------------|---------------------------|---|---|
| 25806.5369    | 0.0005                    | 1 | 2 | 41041.0343    | 0.0008                    | 4 | 11|
| 34013.9166    | 0.0004                    | 5 | 12| 41361.1040    | 0.0006                    | 4 | 9 |
| 35117.9541    | 0.0004                    | 5 | 6 | 41403.0150    | 0.0005                    | 2 | 9 |
| 38467.2068    | 0.0007                    | 2 | 9 | 41529.3210    | 0.0011                    | 2 | 9 |
| 38932.6334    | 0.0016                    | 2 | 8 | 41585.5483    | 0.0014                    | 2 | 10|
| 39243.1896    | 0.0004                    | 2 | 9 | 41745.4442    | 0.0006                    | 4 | 11|
| 39506.7468    | 0.0006                    | 1 | 2 | 42003.4633    | 0.0012                    | 3 | 8 |
| 39640.1103    | 0.0011                    | 2 | 10| 42237.8531    | 0.0008                    | 3 | 8 |
| 39887.8122    | 0.0007                    | 2 | 8 | 42265.6466    | 0.0012                    | 4 | 9 |
| 40027.2324    | 0.0007                    | 3 | 9 | 42613.6123    | 0.0014                    | 2 | 7 |
| 40100.1245    | 0.0009                    | 3 | 14| 42901.2523    | 0.0008                    | 3 | 8 |
| 40300.0712    | 0.0006                    | 4 | 11| 43487.4820    | 0.0017                    | 4 | 12|
| 40491.3398    | 0.0005                    | 3 | 10| 44153.5692    | 0.0005                    | 2 | 8 |
| 40933.9985    | 0.0004                    | 3 | 4 | 9 |

### Notes.
New ThI and ThII energy levels, as determined from coincident sums between the known energy levels and the unclassified lines of Th. N is the number of lines used to determine each level.

Prior to the level optimization we modified the wavenumber and uncertainties from some of the literature sources, as described below.

1. **GBCZ74.** The uncertainties of the individual lines are not reported, but they report an average difference between their measured wavenumbers and calculated Ritz wavenumbers of 0.0016 cm⁻¹. We find that the standard deviation between the published wavenumbers and the Ritz wavenumbers is 0.0034 cm⁻¹, and it is this value that we assigned as an uncertainty for all lines in GBCZ74.

2. **ZC74, Z76.** The lines reported in both ZC74 and Z76 come from several sources, and thus it is not too surprising that the uncertainties and systematic errors vary throughout these...
We did not modify the wavenumbers of these measurements. The wavenumber uncertainties of these lines were described as being less than 0.001 cm\(^{-1}\) for the brightest lines, but no individual uncertainties, nor the calibration uncertainty, were published. In order to estimate the calibration uncertainty, we downloaded the spectrum from the NSO data archive\(^5\) and redetermined the wavenumber correction factor using the argon standards of Whaling et al. (2002) with the corrections of Sansonetti (2007). We found the wavenumber correction factor to be \((-7.09 \pm 0.05) \times 10^{-7}\), which is consistent with the published wavenumber correction factor of \(-7.06 \times 10^{-7}\). Based on a comparison to the Ritz wavelengths, we estimated the uncertainties using Equation (7), where \(c = 0.00107\) and \(d = 0.242\).

5. LP07. A comparison between the LP07 lines and the corresponding PE83 lines suggests that the uncertainties of LP07 were underestimated by a factor of almost 7. We estimated the uncertainties of LP07 using Equation (7), with \(c = 0.0796\) and \(d = 0.310\) (and no wavenumber correction factor). Only LP07 lines that were not found by PE83 were included in the level optimization.

6. KNS08. Neither the wavenumbers nor the wavenumber uncertainties of these measurements were modified.

7. New measurements (RNS13). Neither the wavenumbers nor the wavenumber uncertainties presented in Table 1 were modified.

The classified line lists for Th\(\text{I}\), Th\(\text{II}\), and Th\(\text{III}\), including these modifications, were taken as input to the program LOPT (Kramida 2011). This program performs a least-squares level optimization to produce improved level values and uncertainties. It also calculates Ritz wavelengths based on the new level values with uncertainties based on the variance and covariance of the combining levels.

Having established improved values for the known levels, we searched for new energy levels using the unclassified thorium lines from PE83, EHW03, KNS08, and RNS13. The known energy levels were taken in groups that included levels of a single parity and ionization stage with three adjacent \(J\) values. The unknown lines were summed and differenced with the known levels, producing a large list of potential new level values. This list was sorted by energy and searched for coincident values.

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### Table 5

Newly Identified Neon Lines from PE83

| PE83 Wavenumber (cm\(^{-1}\)) | PE83 Uncertainty (cm\(^{-1}\)) | Observed Neon Wavenumber (cm\(^{-1}\)) | Observed Neon Uncertainty (cm\(^{-1}\)) | Ritz Wavenumber (cm\(^{-1}\)) | Ritz Uncertainty (cm\(^{-1}\)) | Source(s) | Neon Ion | Note |
|-------------------------------|-------------------------------|---------------------------------------|---------------------------------------|-------------------------------|-------------------------------|-----------|---------|------|
| 7839.3225                     | 0.0008                        | 7839.3186                             | 0.0014                                | 7902.5221                     | 0.0012                        | SBS04     | Ne\(\text{I}\) | o    |
| 7902.5344                     | 0.0009                        | 7902.5212                             | 0.0005                                | 7902.5221                     | 0.0012                        | Q94, KN06 | Ne\(\text{II}\) | o    |
| 8020.8325                     | 0.0007                        | 8020.8372                             | 0.0014                                | 8020.8325                     | 0.0014                        | SBS04     | Ne\(\text{I}\) | o    |
| 8975.4635                     | 0.0008                        | 8975.4657                             | 0.0015                                | 8975.4635                     | 0.0015                        | SBS04     | Ne\(\text{I}\) | o    |
| 10992.9246                    | 0.0009                        | 10992.9150                            | 0.0006                                | 10992.9263                    | 0.0004                        | P71, KN06 | Ne\(\text{II}\) | r    |
| 11214.1595                    | 0.0023                        | 11214.1400                            | 0.0003                                | 11214.1666                    | 0.0004                        | P71, KN06 | Ne\(\text{II}\) | o    |
| 11280.4026                    | 0.0024                        | 11280.4000                            | 0.0003                                | 11280.4024                    | 0.0015                        | P71, KN06 | Ne\(\text{II}\) | r    |
| 11383.7990                    | 0.0009                        | 11383.7997                            | 0.00010                               | 11383.7997                    | 0.00010                       | SBS04     | Ne\(\text{I}\) | o    |
| 11483.7423                    | 0.0020                        | 11483.7600                            | 0.0003                                | 11483.7430                    | 0.0003                        | P71, KN06 | Ne\(\text{II}\) | r    |
| 11517.0622                    | 0.0014                        | 11517.0900                            | 0.0020                                | 11517.0623                    | 0.0033                        | P71, KN06 | Ne\(\text{II}\) | r    |

Notes. A subset of PE83 wavenumbers that correspond to neon lines. Revisions to the wavenumbers and uncertainties of the PE83 lines are described in the text. Literature values for the Ne\(\text{I}\) lines are taken from the compilation of Saloman & Sansonetti (2004), while those of Ne\(\text{II}\) are from Kramida & Nave (2006). The source identifications are as follows: MH2, Meggers & Humphreys (1934); BAL, Burns et al. (1950); EHR, Ehrhardt (1970); P71, Persson (1971); PE83, Palmer & Engleman (1983); SBS04, Sansonetti et al. (2004); and KN06, Kramida & Nave (2006). The last column indicates whether the line matches the observed wavenumber (o) or the Ritz wavenumber (r). Lines without a comment in this column match both.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)
## Table 6
Thorium Line List

| Ritz Wavenumber (∙ cm⁻¹) | Ritz Wavenumber Uncertainty (δσ) (cm⁻¹) | Ritz Vacuum Wavelength (λ) (Å) | Ritz Vacuum Wavelength Uncertainty (δλ) (Å) | Species | Relative Intensity | Odd Energy (cm⁻¹) | Even Energy (cm⁻¹) | Measured Wavenumber (cm⁻¹) | Measured Wavenumber Uncertainty (cm⁻¹) | Source | Note |
|------------------------|----------------------------------------|-----------------------------|---------------------------------------------|--------|-----------------|-----------------|-----------------|---------------------|-------------------------------|--------|------|
| 9816.11445             | 0.00010                                | 10187.33028                 | 0.00011                                     | Thⅰ   | 180             | 23113           | 4               | 13297               | 4                             | 9816.1146 | 0.0004 | PE83 |
| 9819.6098              | 0.0003                                 | 10183.7040                  | 0.0003                                      | Thⅰ   | 0               | 17837           | 1/2             | 08018               | 3/2                           | 9819.616   | 0.003 | GBCZ74 |
| 9819.91929             | 0.00006                                | 10183.38309                 | 0.00006                                     | Thⅰ   | 290             | 17224           | 2               | 27044               | 3                             | 9819.91911 | 0.0003 | PE83 |
| 9821.92006             | 0.00005                                | 10181.30868                 | 0.00005                                     | Thⅰ   | 1500            | 22669           | 3               | 12847               | 3                             | 9821.92015 | 0.00011 | PE83 |
| 9823.30548             | 0.00020                                | 10179.87277                 | 0.00020                                     | Thⅰ   | 37              | 28372           | 1               | 18549               | 2                             | 9823.3059  | 0.0011 | PE83 |
| 9825.30957             | 0.00006                                | 10177.79636                 | 0.00006                                     | Thⅰ   | 1200            | 14206           | 4               | 24032               | 4                             | 9825.30956 | 0.00012 | PE83 |
| 9830.8247              | 0.0004                                 | 10172.0866                  | 0.0004                                      | Thⅰ   | 59              | 28932           | 4               | 38763               | 5                             | 9830.8230  | 0.0008 | PE83 |
| 9830.82333             | 0.00019                                | 10172.08800                 | 0.00020                                     | Thⅰ   | 59              | 20686           | 5/2             | 10855               | 7/2                           | 9830.8230  | 0.0008 | PE83 |
| 9839.51266             | 0.00010                                | 10165.10497                 | 0.00010                                     | Thⅰ   | 380             | 25703           | 2               | 15863               | 2                             | 9839.512   | 0.003 | Z76  |
| 9843.30405             | 0.00011                                | 10159.19040                 | 0.00011                                     | Thⅰ   | 33              | 19039           | 2               | 28882               | 2                             | 9843.3041  | 0.0011 | PE83 |
| 9855.08606             | 0.00003                                | 10147.04483                 | 0.00003                                     | Thⅰ   | 720             | 16217           | 2               | 06362               | 2                             | 9855.08586 | 0.00016 | PE83 |

Notes. A sample of the compiled thorium line list. The energy levels have been rounded down to an integer. The actual values of the energy levels can be found in Table 7. GBCZ74, Giacchetti et al. (1974); ZC74, Zalubas & Corliss (1974); Z76, Zalubas (1976); PE83, Palmer & Engleman (1983); EHW03, Engleman et al. (2003); LP07, Lois & Pepe (2007); KNS08, Kerber et al. (2008); RNS13, this publication. An “A” in the last column indicates a measured line that matches more than one classification. A “B?” indicates a line that deviates from the Ritz wavenumber by 5 or more times its measured uncertainty, and therefore was not included in the level optimization.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)
produced by multiple combinations of lines and levels that might signal a new level with the opposite parity and central J value. Because of the high density of potential level values, the likelihood of accidental coincidences is large. To assess the validity of accepting a new level based on a particular number of coincident predictions, we ran Monte Carlo simulations to determine the number of coincident sums and differences that would be expected to occur by chance. For each ionization stage and combination of adjacent J values, we performed 200 simulations, adding a uniformly distributed random amount between $-0.1 \text{ cm}^{-1}$ and $0.1 \text{ cm}^{-1}$ to the unidentified lines. Only new energy levels with a probability of <0.01 of being coincidences were included. Based on these results, we have accepted 93 new Th I energy levels and 9 new Th II energy levels. Details of the new levels are given in Table 4. We were not able to constrain the J value of several of these lines; in these cases, the two or three possible J values are provided.

Using compilations of neon lines from Saloman & Sansonetti (2004) and Kramida & Nave (2006), we found 69 PE83 lines that were better matches to neon lines than to thorium Ritz wavelengths. In all cases, these lines have larger line widths than the nearby thorium lines, as would be expected for the gas lines. PE83 only reported their line widths in a machine-readable table, which is not publicly available. This table also includes many faint lines that were not included in their published atlas. The PE83 measurements for lines we have identified as neon are usually more accurate than any previously reported measurements in the literature. They are presented in Table 5.

Our final list of classified thorium lines is provided in Table 6. This list includes 227 multiply classified lines and 71 lines from PE83, EHW03, KNS08, and RNS13 with large discrepancies between their measured and Ritz wavenumbers that were not used in the level optimization. The first column is the Ritz wavenumber, which can be used for wavelength calibration and will usually be more accurate than the measured wavenumber. The second column is the Ritz wavenumber uncertainty as determined by the variance and covariance of the level optimization in LOPT. The third and fourth columns are the corresponding Ritz wavelength and uncertainty. The fifth column indicates that the difference between the measured and Ritz wavenumber is more than five times the measured uncertainty of the line, and therefore was not included in the level optimization. The second-to-last column provides the source for the measured wavenumber. An “A” in the final column indicates that the line matches more than one thorium Ritz wavenumber. An “B” in the final column indicates that the difference between the measured and Ritz wavenumber is more than five times the measured uncertainty of the line, and therefore was not included in the level optimization.

In order to help guide users of this line list, we have estimated the relative intensities of the lines by matching lines from the different line lists and adjusting their intensities so that they are all on approximately the same scale. Placing all line lists on the same intensity scale is complicated by the fact that the

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**Table 7**

Optimized Thorium Energy Levels

| Energy (cm$^{-1}$) | Uncertainty (cm$^{-1}$) | J | N | Energy (cm$^{-1}$) | Uncertainty (cm$^{-1}$) | J | N | Energy (cm$^{-1}$) | Uncertainty (cm$^{-1}$) |
|-------------------|-------------------------|---|---|-------------------|-------------------------|---|---|-------------------|-------------------------|
| 0.000000         | 0.000100               | 2 | 189 | 46902.5368      | 0.0011          | 5/2 | 22 | 7176.10661     | 0.0003          | 2 | 10 |
| 2558.05675       | 0.000108               | 0 | 48  | 1521.89632      | 0.00010          | 5/2 | 80 | 63.26679      | 0.0003          | 2 | 9 |
| 2869.25916       | 0.00017                | 3 | 198 | 1859.93843      | 0.00011          | 3/2 | 60 | 7875.8244     | 0.0004          | 1 | 5 |
| 3687.98718       | 0.00013                | 1 | 181 | 4113.35932      | 0.00011          | 5/2 | 75 | 9953.58098    | 0.0003          | 3 | 12 |
| 3865.47737       | 0.00016                | 1 | 126 | 4146.57708      | 0.00011          | 7/2 | 70 | 10440.2372    | 0.0004          | 2 | 6 |
| 4961.65883       | 0.00019               | 4 | 176 | 27631.2250      | 0.00024          | 3/2 | 20 | 10542.8987    | 0.0003          | 4 | 9 |
| 5563.14151       | 0.00016               | 1 | 114 | 27937.0722      | 0.0003          | 11/2 | 17 | 11961.1316    | 0.0007          | 0 | 3 |
| 6362.39598       | 0.00016               | 2 | 183 | 28011.1578      | 0.0003          | 3/2 | 13 | 15148.5193    | 0.00023         | 4 | 10 |
| 7280.12322       | 0.00023               | 2 | 179 | 28026.3485      | 0.0005          | 5/2 | 18 | 16037.6412    | 0.0003          | 2 | 9 |
| 7502.28763       | 0.00016               | 3 | 184 | 28823.6538      | 0.00025         | 5/2 | 23 | 17887.4092    | 0.0003          | 5 | 7 |

**Notes.** A subset of the compiled Th I (left), Th II (center), and Th III (right) energy levels. The even levels are in the top half of the table, and the odd levels are in the bottom half of the table.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)
ratio between line intensities from different line lists vary as a function of wavenumber. It is also important to note that different lamp currents could greatly alter the relative intensities of lines from the values published here (e.g., Kerber et al. 2006). We estimate that these intensities are only good to an order of magnitude.

Our re-optimized energy levels for Th i, ii, and iii are presented in Table 7. The level uncertainties are with respect to the ground state as determined by LOPT. The first column is the energy of the level, and the second is its uncertainty. The third column provides the J value of the level, and the fourth column indicates the number of measured spectral lines that were used to determine the energy level. These energy level uncertainties are in general an order-of-magnitude better than previously reported level uncertainties.

4.1. Implications for Astronomical Measurements

Our new line list contains the most accurate wavelengths of the thorium spectrum measured to date. There are two major astrophysical applications that will benefit from this line list: precise radial velocity measurements and measurements of the fine-structure constant as a function of redshift.

Precise radial velocity measurements (such as those made with the HARPS spectrograph) rely on relative wavelength shifts. More accurate wavelengths can only improve the measured dispersion solution, but the size of the improvement will depend on the resolution of the spectrometer, the correction of systematic errors, and the instrumental line profile. Our line list will provide the most significant improvement to the dispersion solutions of high-resolution instruments that were previously utilizing the thorium line list of LP07. We note that these improved wavelengths should help characterize the systematic errors of CCDs and infrared arrays, such as those discovered on the HARPS spectrograph by Wilken et al. (2010).

On the other hand, measurements of the fine-structure constant (α) rely upon absolute thorium and argon wavelengths to accurately measure slight changes in the value of α as a function of redshift (Murphy et al. 2003). Systematic changes in the thorium wavelengths can significantly alter the significance of the measured result. This is demonstrated very nicely by Figure 11 of Murphy et al. (2007), which shows an example of how changes in the thorium wavelengths can transform a published null result into a possible detection at the level of 2.5 sigma. We note that Murphy et al. (2007) utilized LP07 thorium wavelengths to solve the dispersion solution of the Very Large Telescope Ultraviolet and Visual Echelle Spectrograph. It is not easy for us to predict how the application of our line list will affect the measured changes in α, since such an application depends on the exact lines used to solve the dispersion solution and their proximity to the redshifted quasar absorption lines.

5. CONCLUSIONS

We have compiled a new thorium line list based on the values from seven previously published sources and our new measurements from the 2 m FTS at NIST. Using these data, we re-optimized the energy levels of neutral, singly, and doubly ionized thorium and calculated a list of 19,874 Ritz wavelengths between 250 nm and 5500 nm. We included in the list only lines that have been observed experimentally. An additional 227 lines have ambiguous classifications and another 71 lines marginally matched a Ritz wavenumber, but have been included in the list for completeness. We consider the Ritz wavelengths from this list to be suitable for use as calibration standards for new and archival thorium spectra recorded with high-resolution spectrometers.

This research was performed while S. Redman held a National Research Council Research Associateship Award at NIST.

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