



Development of an In-House Grating Spectrometer System for Validating Acousto-Optic Tunable Filter Spectrometer Results

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Abstract

We describe the design of a grating spectrometer system. We obtained emission spectroscopy results of a lamp source from a visible to near infrared (vis-NIR) acousto-optic tunable filter (AOTF) spectrometer and from an IN-house developed Grating (ING) spectrometer. We compare the measured lamp source emission-spectra results from the grating spectrometer with results obtained with the AOTF spectrometer and results from the lamp manufacturer. The grating spectrometer compares well with the manufacturer's calibrated data and results obtained from the AOTF spectrometer.

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1. Introduction

The Army Research Laboratory (ARL) has performed various spectroscopy measurements, including laser and UV-induced fluorescence, Raman, absorption, and emission using acousto-optic tunable filter (AOTF) spectrometers [1]. The use of AOTF spectrometers to make such measurements, along with novel measurement techniques and setup, makes chemical detection possible at very low concentration levels. The monitoring of water pollutants and the detection of explosives have been successfully performed at ARL with AOTF spectrometers [2,3]. Unique spectral signatures have been obtained for different chemical compounds; some of these have very similar Raman signatures but an AOTF spectrometer was able to isolate them.

To verify the performance and characterize the spectroscopy results obtained with AOTF spectrometers, we need to calibrate the AOTF spectrometers with results obtained from a traditional grating spectrometer. To do this, we coupled a SPEX 500M monochromator with a photomultiplier tube (PMT) detector, low-noise current amplifier, and computer interface with GPIB (general purpose interface bus) and DAQ (digital acquisition) capability to develop a computer-controlled plane-grating-type spectrometer (the IN-house Grating or ING spectrometer). We developed LabVIEW software to control the operations of the spectrometer including instrument control, digital acquisition, and file handling.

We describe the design and development of the grating-based spectrometer with emphasis on the system development and software design. We will present emission spectroscopy results obtained from a PEN-RAY[®] argon lamp source with the use of both the ING and vis-NIR AOTF spectrometers.

2. Description of ING Spectrometer System

The ING spectrometer system is comprised of the components shown in figure 1. The SPEX 500M monochromator (fig. 2) allows only a very narrow band of wavelengths of light to pass through the exit slit by diffracting the incoming light with the use of a plane grating. Light enters the entrance slit (see fig. 3) and is collected by a collimating mirror that uniformly spreads the light onto a plane grating. The diffracted light from the plane grating is then collected by a second mirror that focuses the diffracted light at the exit slit. If the incoming light is monochromatic, then only that wavelength of light will pass through the exit slit when the grating is in the proper position, corresponding to that wavelength of light. If a broad spectrum of light enters the entrance slit at the same time (e.g., a white light source), then several diffracted wavelengths of light will strike the exit plane, but only one wavelength of light will pass through the exit slit, depending on the grating position. A scan motor is used to correctly position the grating of the monochromator.

Figure 1. Block diagram of grating spectrometer.

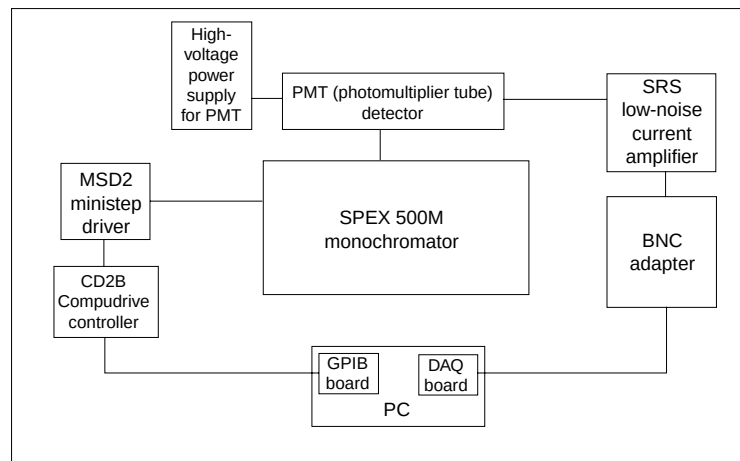
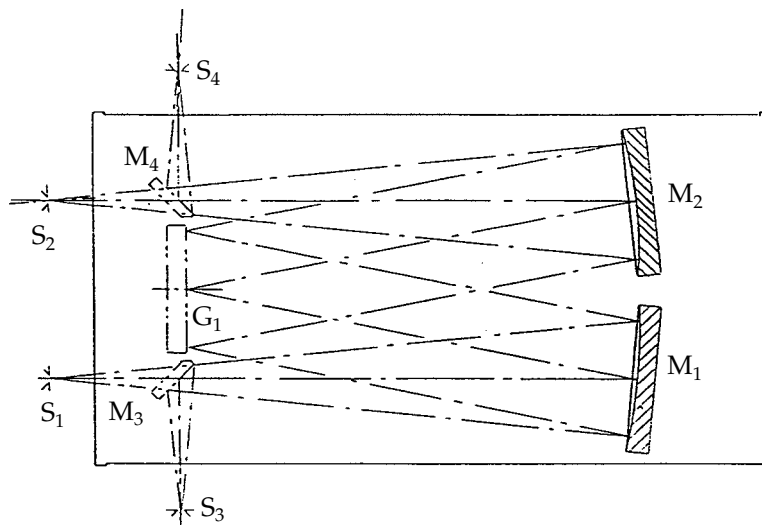


Figure 2. SPEX 500M monochromator.



Figure 3. Optical diagram of SPEX 500M monochromator.



After the light exits the exit slit of the monochromator, it strikes the detector. In this case, the detector is a PMT. The PMT creates an electrical current proportional to the number of photons striking the light-sensitive cathode of the PMT (photoemission). The electrical current is multiplied by electrons striking the surface of the successive dynode stages of the PMT at very high dc voltage potentials created by an external high-voltage dc power supply.

The electrical current coming out of the PMT is amplified by a low-noise current amplifier that provides low bandpass filtering for high-frequency noise reduction, signal amplification, and selectable current-to-voltage conversion ranging from 1 pA/V to 1 mA/V.

The output of the current amplifier is connected to a BNC analog connector interface box for interfacing the analog signal with a DAQ board inside the PC. Once the DAQ board receives the analog signal, the voltage is digitized into one of 4096 digital voltage levels.

A ministep driver (MSD2) controls the scan motor of the monochromator. The ministep driver is controlled by the CompuDrive controller (CD2B), which in turn can be controlled through front panel inputs or from a remote device controller (PC) through a GPIB interface. A GPIB interface card inside the PC is used to establish the remote device controller interface. We wrote software in LabVIEW to provide a user-friendly interface that would enable the effective and efficient use of the spectrometer to its fullest potential.

3. LabVIEW Software

The LabVIEW software links the instrument control with the DAQ to provide a very user-friendly environment for operating the ING spectrometer. This environment allows complete interactive control of the ING spectrometer. Unlike a single-line command-driven menu environment, input parameters and action commands can be changed at any time prior to execution, and certain commands and actions can be changed while the software is executing. Software indicators allow the user to easily determine when a feature is being implemented, and software switches allow a user to enable or disable a feature easily. Many of the switches and indicators blink and change color to alert the user as to the status of the measurements and to indicate when a decision or action needs to be made. In terms of error correction, the LabVIEW environment allows easy detection and correction of software or hardware problems, making for an extremely flexible and powerful operating environment.

The front panel (see appendix) design closely matches the CD2B Compdrive input panel for logical input flow. Input parameters include:

1. Wavelength start and stop position,
2. Wavelength scan rate,
3. Number of scans for averaging,
4. Scan delay for delaying the beginning of a scan when not in trigger scan mode,
5. Dwell time for pausing between wavelength scan increments when burst mode is selected and trigger scan is off,
6. Scan mode for burst or continuous scanning operation,
7. Continuous operation selection for continuous execution of selected parameter set, and
8. High- and low-voltage selection for digital acquisition.

The software provides graphing of the data, displaying individual values at a given wavelength, averaging of several scans, displaying the averaged scans and the last scan simultaneously, and file saving capability. The LabVIEW graphing software has a zoom-in feature that causes resolution changes in the vertical and horizontal axis to allow detection of small peaks in a spectrum that otherwise may not be noticeable. The file saving part of the software allows the user to save the data for use in a spreadsheet (such as Microsoft Excel) or other graphing software. The software also allows the user to easily perform calibration of the grating spectrometer. Instruments SA, Inc./SPEX calibrated the grating spectrometer using the LabVIEW software we developed.

4. Results and Discussion

The grating spectrometer was calibrated and realigned to system specifications by a SPEX field engineer using a green He-Ne laser operating at 5460.74 Å along with the developed LabVIEW software. After realignment and calibration, the measured resolution was 1 Å at 5460.74 Å and the wavelength accuracy of the instrument was approximately ± 1 Å at a measured wavelength of 5459.6 Å.

We obtained emission spectroscopy results for the PEN-RAY argon lamp source using both the ING and vis-NIR AOTF spectrometers. Figures 4(a) and (b) show the emission spectrum of the argon lamp source measured with the ING spectrometer from 3200 to 4400 Å and 6700 to 8000 Å, respectively. The measurements in figure 4 were made with an entrance slit width to the ING spectrometer of 0.012 mm, a current amplifier set for low-noise gain with a lowpass filter cutoff frequency of 30 Hz, and a PMT voltage of 1.25 kV dc. Figure 5 shows the emission spectrum of the argon lamp source measured with the vis-NIR AOTF spectrometer. For the results shown in figure 5, the vis-NIR AOTF spectrometer parameters (points per scan range for resolution, number of scans for averaging, current amplification, and PMT dynode voltage) were varied to give the best results with respect to spectral resolution, sensitivity, and signal-to-noise ratio (SNR). Comparing the results between the two spectrometers shows that the spectra are very similar. Both spectrometers detect the same lines with very similar peak intensities relative to the other lines. Differences in relative peak intensity between the two systems may be attributed to the differences in spectral resolution of the two systems. The results obtained with the larger spectral resolution AOTF spectrometer (4 to 5 Å at 6700 to 8000 Å) were relatively lower in intensity than those obtained with the ING spectrometer (~ 1 Å) because the narrow peaks are averaged over 4 to 5 Å as opposed to ~ 1 Å resolution. In general, however, if the narrow peaks had an FWHM (full width at half maximum) much less than 4 to 5 Å in the 6700 to 8000 Å range, the peaks may have been undetectable with the AOTF spectrometer.

We placed neutral density (ND) filters in front of the lamp source to determine if the observed measured peaks were being generated as a result of only the lamp source and not some other source of light. If the intensity of a given peak reduces by a factor corresponding to the ND filter selected, the intensity peak can be considered as coming from only the lamp source. If an intensity peak resulted from an unknown light source, noise, or other unknown or random contributions, then the resultant peak would not track with the ND filter, and therefore, the intensity peak could be considered a false result. Figures 6(a) and (b) show results of an argon lamp source with the use of an ND filter with an O.D. of 0.3, which reduces the light transmission coming from the lamp source by a factor of 2 for the ranges of 3200 to

Figure 4. Emission spectrum of argon lamp source using ING spectrometer from (a) 3200 to 4400 Å and (b) 6700 to 8000 Å.

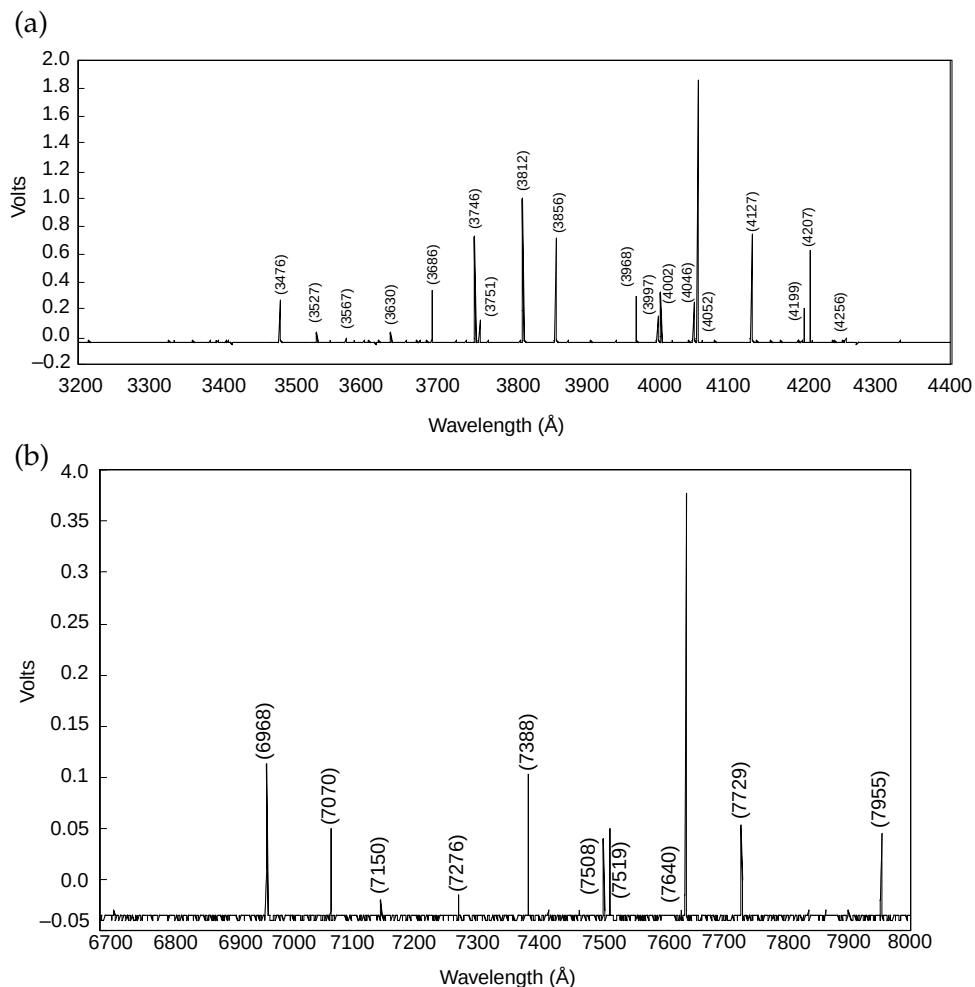
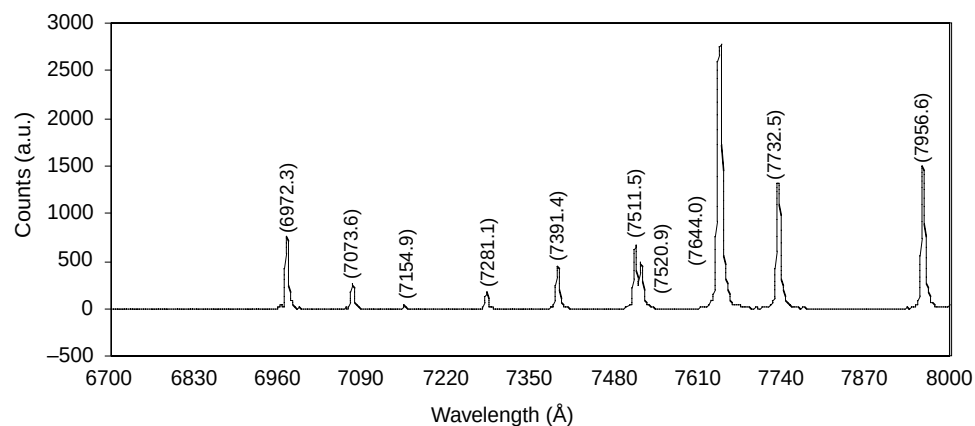
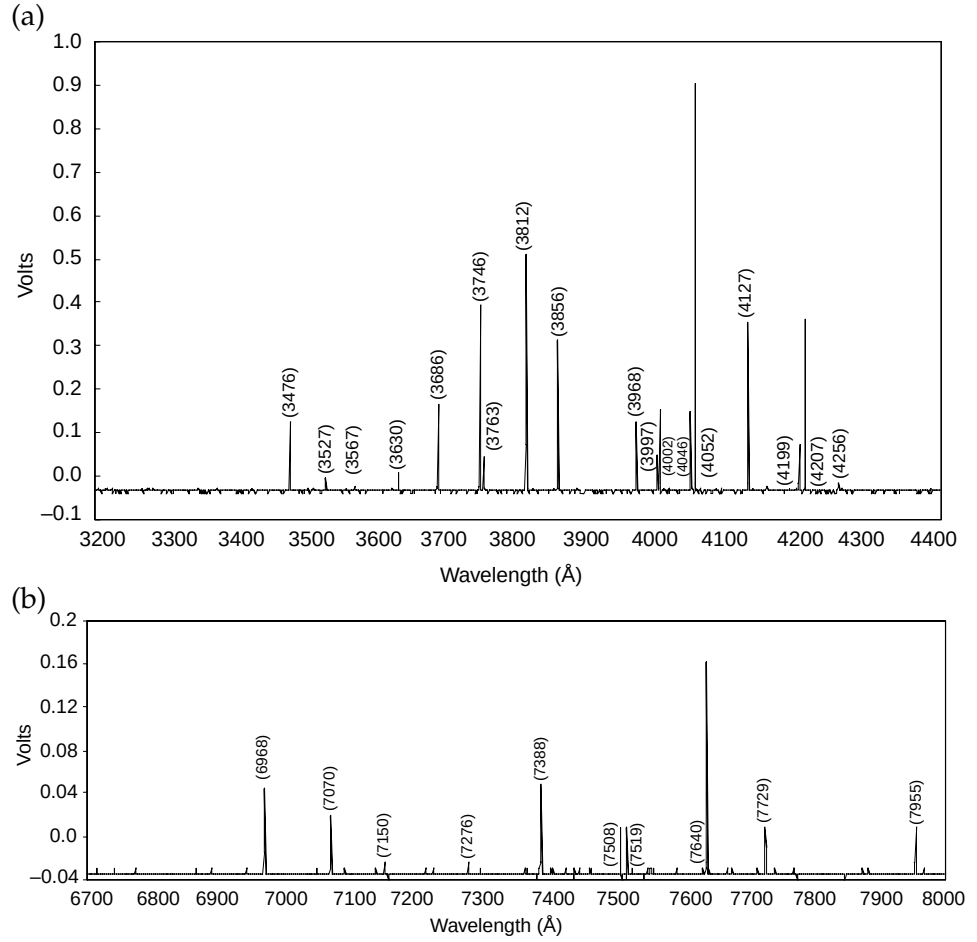


Figure 5. Emission spectrum of argon lamp source using AOTF visible-to-near infrared (NIR) spectrometer from 6700 to 8000 Å.



4400 Å and 6700 to 8000 Å, respectively. As this figure shows, the intensity peaks are reduced by a factor of approximately 2, compared with the results shown without any ND filter (fig. 4). Therefore, the results obtained without any filter can be considered a true spectrum of the measured lamp source.

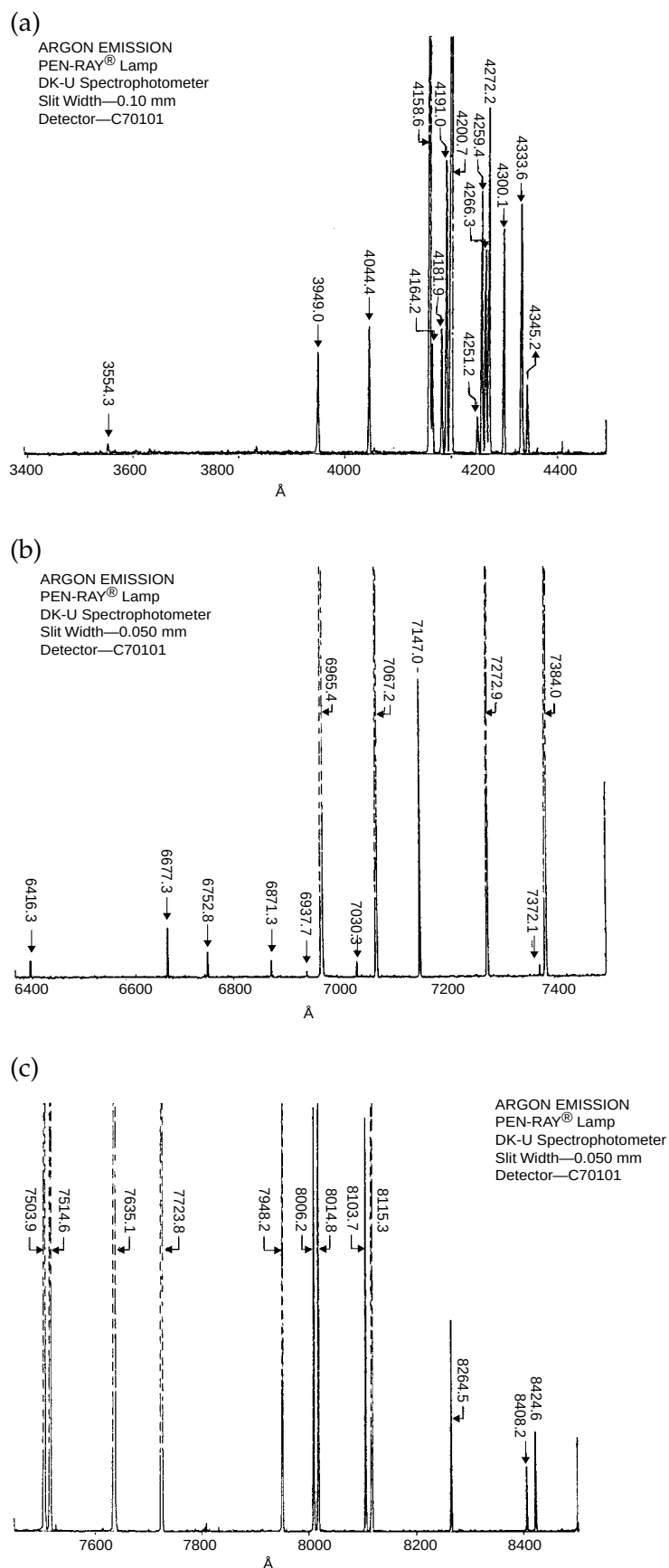
Figure 6. Emission spectrum of argon lamp source with a neutral density filter used to reduce light transmission into ING spectrometer by a factor of 2 from (a) 3200 to 4400 Å and (b) 6700 to 8000 Å.



A noticeable difference between the results of the ING and vis-NIR AOTF spectrometers is the superior resolution capability of the former over the latter. With the ING spectrometer, at wavelengths 7505 and 7519 Å for the argon lamp source, two distinct, separate peaks that do not overlap result. But the AOTF spectrometer is not able to separate the two peaks and an overlap results. Moreover, if the two peaks had been closer to each other, the AOTF spectrometer may not have been able to resolve any distinction between them. The ING spectrometer results show its superior spectral resolution (~ 1 Å) compared to the vis-NIR AOTF spectrometer (1 to ~ 5 Å from 4000 to 8000 Å). This is more evident at higher (longer) wavelengths (6000 to 8000-Å range) where the spectral resolution of the vis-NIR AOTF spectrometer is greater.

The emission spectrum of the PEN-RAY argon lamp published by the manufacturer is shown in figures 7(a), (b), and (c) for the wavelength ranges from 3400 to 4400, 6400 to 7400, and 7500 to 8500 Å, respectively. The manufacturer's results were measured using a Beckman DK-U spectrometer [4] with an entrance slit width of 0.050 mm in combination with a scanning grating monochromator and an RCA tri-alkali detector C70101. The major lines shown in figure 7(b) (7384.0, 7272.9, 7067.2, and 6965.4 Å) are detected by the other two spectrometers (ING and vis-NIR AOTF). However,

Figure 7. Emission spectrum of PEN-RAY argon lamp source from (a) 3400 to 4400 Å, (b) 6400 to 7400 Å, and (c) 7500 to 8500 Å. Reproduced by permission of UVP, Inc.



many of the lines shown in figure 7 are not present in either of the results obtained by the ING and vis-NIR AOTF spectrometers. Additionally, variations in intensity also exist between the data from the lamp manufacturer and the data taken with the ING and vis-NIR AOTF spectrometers. Variations in intensity as well as the absence of certain lines could be the result of one or more of the following:

1. Differences in the optical systems (ING versus Beckman DK-U spectrometer) used to make the measurements,
2. Differences in excitation conditions between the two PEN-RAY argon lamps,
3. Differences in electronic processing of the detector output (amplifier gain and filtering),
4. Different detector sensitivity levels (increase in SNR) resulting in detector output variations,
5. Different PMT voltages resulting in detector output variations,
6. Different measuring techniques that may result in variations in sensitivity, and
7. Variations in the source itself, that is, a faulty lamp source may have been used in the measurements with the ING and vis-NIR spectrometers that would explain the missing lines in the spectra taken with these instruments [5].

5. Summary

The ING spectrometer provides a user-friendly environment with many features (file saving to spreadsheet formats such as Excel, graphing, averaging, different scanning modes, easier calibration of instrument) that make it a very useful tool for comparing results obtained with AOTF spectrometers.

Emission spectroscopy results of a PEN-RAY argon lamp source with the use of the ING spectrometer are comparable to the manufacturer's lamp source calibration data and measurements obtained by the vis-NIR AOTF spectrometer.

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Appendix. Front Panel Diagram of LabVIEW Code Developed for the ING Spectrometer

The entire LabVIEW software code is available upon request.

Parameters

START POSITION
[]

END POSITION
[]

SCAN RATE
[]

NUMBER OF SCANS
[1]

SCAN DELAY
[0]

DWELL TIME
[0]

GPIB Address
[10]

Mode

SCAN TYPE
[B]

Commands

Trigger Scan
ON OFF

High Limit
[0.00]

Low Limit
[0.00]

Save File ?
YES

Perform File Action
DOIT

XY Graph

0.5
0.0
-0.5

7600.0 7650.0

Data 1
Data 2

Continuous Operation
OFF ON

File Saving Instructions
None.

Position Array
[0] [0.00] [0.00] [0.00]

Avg. Intensity Array
[0] [0.00] [0.00] [0.00]

Intensity Array
[0] [0.00] [0.00] [0.00]

GO

Present Position
[]

Present Scan Number
[0]

Total Number of Scans
[0]

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