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Application News

UV-Vis Spectrophotometer UV-2600i

Standard Test Method for Quantifying Naphthalene with UV-2600i Ultraviolet Spectrophotometer: ASTM D1840

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User Benefits

- ASTM D1840 for quantifying naphthalene hydrocarbons in aviation fuels by ultraviolet spectrophotometry, addressing industry demands for greater regulation on the compound.
- The UV-2600i provides great versatility in the examination of di-aromatics in solution, performing spectroscopic measurements required in the test method with high precision.
- LabSolutions's UV-Vis software simplifies detection of naphthalene's characteristics with features such as peak point identification and construction of a calibration curve within quantitative measurement mode.

■ Background

Aviation fuels are composed of a mixture of hydrocarbons and additives specific to the use of the fuel. Aromatic components found in this mixture include, but are not limited to, benzene, naphthalene, and other mono-aromatics[1]. Naphthalene is a white crystalline solid and is considered the simplest and most volatile compound of the polycyclic aromatic hydrocarbon group, having a two six-membered ring structure[2]. In fuel, naphthalene is used as a catalyst for the combustion process and helps to maintain the seal of integrity of the aircraft's fuel system.

The presence of Naphthalene in jet fuels has fallen under examination due to its role in soot emissions. Soot particles are a contributing factor for global warming and air quality degradation, effectively absorbing sunlight, trapping heat, and contributing to haze formation. Furthermore, soot emission is associated with negative impacts on human health through respiratory issues and increased risk of cardiovascular diseases[3]. The American Society for Testing and Materials has produced a standard test method (ASTM D1840) for quantifying naphthalene hydrocarbons in aviation fuels by ultraviolet spectrophotometry, addressing industry demands for greater regulation on the compound[4]. The test method determines the total concentration of naphthalene, acenaphthene, and alkylated derivatives of hydrocarbons in jet fuels. Jet fuel standards currently set a maximum limit of 3% in volume of naphthalene, with an average actual content of 2-3% in jet fuel sold[5].

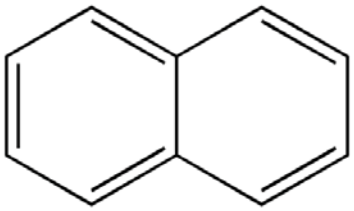

Figure 1: Naphthalene structure is composed of two conjoined benzene rings, C_8H_{10}.

Shimadzu's UV-2600i can perform spectroscopic measurements required in the test method with high precision. User-friendly LabSolutions's UV-Vis software simplifies detection of naphthalene's characteristics within the ultraviolet region through features such as peak point identification and construction of a calibration curve within quantitative measurement mode.

■ Instrumentation

Shimadzu's UV-2600i (Figure 2) was utilized for this study due to its high-absorbance measurement capabilities within the ultraviolet (UV) region. Naphthalene forms a colorless solution in an isooctane solvent, with an absorption spectrum concentration in the UV region. The maximum absorption peak observed during experimentation and used for quantification was 275 nm. All spectral scans performed on samples were acquired as absorption spectral scans, with the spectral range between 200 nm and 400 nm. Further detail on parameters of instrumentation for this study are mentioned in table 1.

Figure 2: Shimadzu's UV-2600i.

Table 1: Parameters for the UV-2600i.

Wavelength (nm)	**Start**	400	**Slit Width**	2.0 nm
	End	200	**Detector Unit**	Direct Receiving of Light
Data Interval		1.0 nm	**Light Source Switch**	315 nm
Scan Speed		Medium speed		
Spectrum Type		Absorbance		

■ Experimental Methods

Following the ASTM D1840[5] test method for naphthalene, serial dilutions were performed with the intention of performing solute analysis (e.g. calibration curve construction and mass percentage calculations). Isooctane, 2,2,4-trimethyl pentane was utilized as the solvent for the dilutions due to the nonpolar nature of the solute. An initial stock solution was formed by weighing 0.5087 g of crystalline powder naphthalene and dissolved with 2,2,4-trimethyl pentane in a 100 mL volumetric flask to form a solution with concentration of 3.97×10^{-2}M. The stock solution was subsequently diluted four times to yield the molar concentrations provided in Table 2.

An additional spectral scan of 2,2,4-trimethyl pentane with no naphthalene solute is referenced as a data point throughout measurements and analysis.

Measurements

Absorbance Measurements with UV-2600i

Spectral scans (Figure 3) were obtained for five concentrations of the naphthalene solution. Utilizing LabSolutions UV-Vis software's point pick feature, absorbance values for each spectral scan were identified. These absorbance values were located at 275 nm, wavelength of the peak maximum (λ_{max}). For all spectral scans, a 1.0 cm path length quartz cuvette was utilized to hold samples. The absorbance values with respect to concentrations are listed in table 2.

Table 2: Sample concentrations and their respective absorbance values at 275 nm.

Absorbance Values and Concentrations		
Sample #	**Concentration (M)**	**Absorbance**
1	6.35×10^{-4}	3.242
2	3.18×10^{-4}	1.554
3	2.54×10^{-4}	1.289
4	6.35×10^{-5}	0.358
5	0.00	0.000

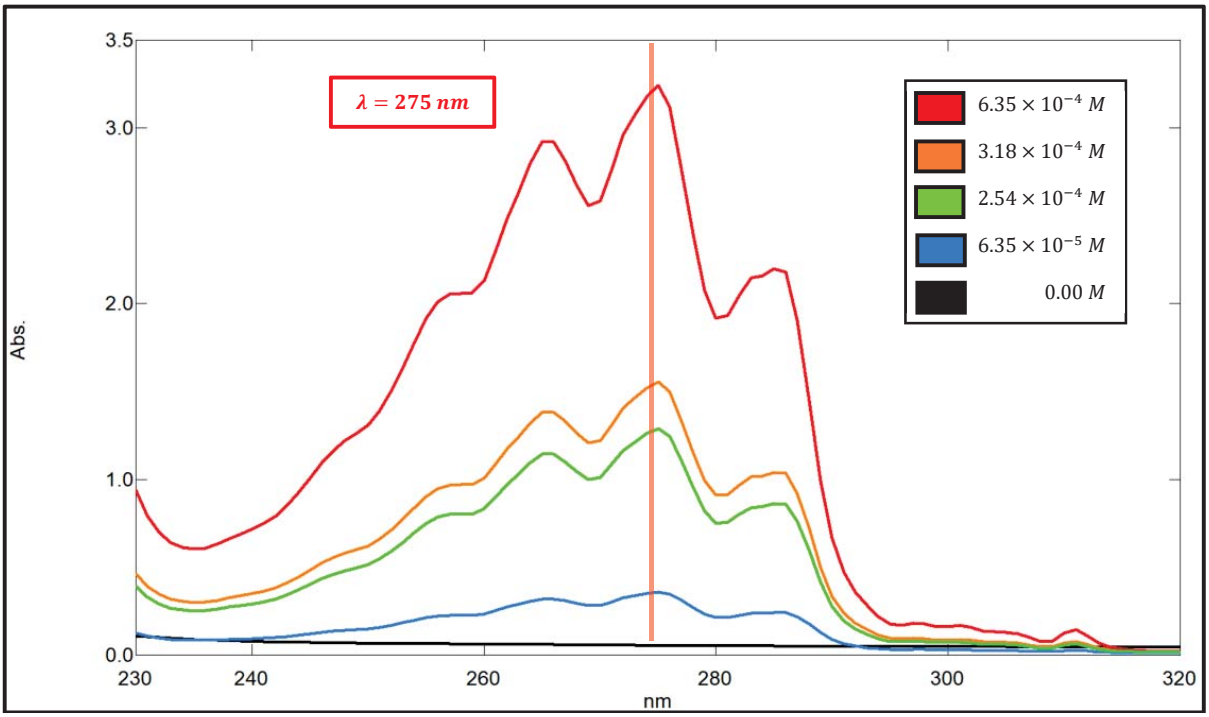

Figure 3. UV-Vis absorption spectra of five naphthalene solutions with concentrations labeled in top right of the spectra. The maximum absorption peak of naphthalene labeled with red line at 275 nm.

Concentration Analysis

Application of Beer-Lambert's Law

Applying Beer-Lambert's law to the serial dilutions performed on naphthalene, the known concentrations and respective absorbance values at the λ_{max} of 275 nm were plotted with a linear fit (Figure 6).

The coefficient of determination of this linear fit was 0.9992.

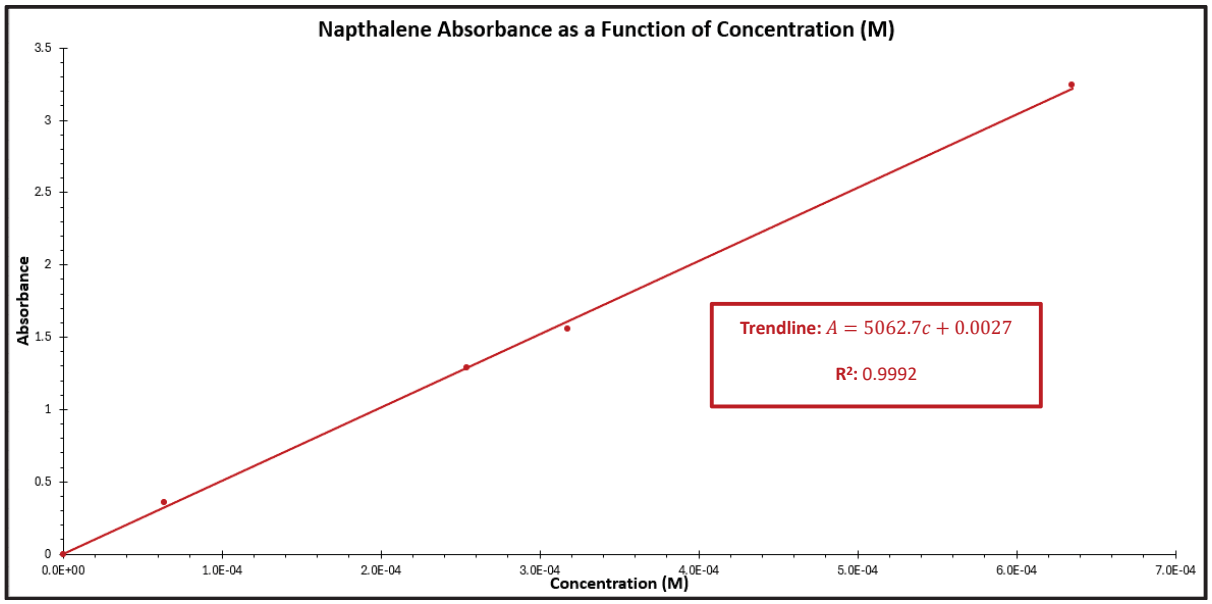

Figure 6: Calibration curve of absorbance as a function of concentration of naphthalene solute. The coefficient 5062.7 represents the molar absorption coefficient of $5062.7 \frac{\mathrm{L}}{\mathrm{mol} * \mathrm{cm}}$, where the optical path length of 1 cm is accounted for within the trendline formula.

Naphthalene Mass Percentage Calculations:

A: Corrected absorbance (observed absorbance minus cell correction) of the dilution measured.
K: Equivalent volume in solvent, in liters, if the dilution had been made in a single step.
W: grams of sample used.

$$\text{Naphthalene, Mass \%} = [\frac{A \times K}{33.7 \times W}] \times 100$$

Figure 7: Formula for determination of the mass percentage of naphthalene in solution.

The mass percentage of naphthalene within samples measured in experimentation was calculated utilizing the formula in Figure 7. Calculations for the mass percentage of naphthalene in solution can be determined with the formula mentioned in the ASTM method[4]. The equation denotes variables such as *A*, *K*, and *W*, which represent properties of the sample. The variable *A* is the corrected absorbance recorded at the λ_{max} wavelength of 275 nm.

Note that a "corrected absorbance" is achieved by performing a baseline with an empty cuvette prior to sample scans. The absorbance values in mass percentage calculations originate from data points found in calibration curve. *K* represents the equivalent volume in liters of solvent needed to reach the dilution in a single step with respect to the original dilution. And *W* representing the weight in grams of naphthalene in solution.

Table 3: Data values utilized to determine the mass percentage of naphthalene in solution.

#	Concentration (M)	Solvent Volume (L)	Sample Mass (g)	Corrected Absorbance	Mass % Naphthalene
1	6.35×10^{-4}	6.25	0.5087	3.242	1.182
2	3.18×10^{-4}	12.48	0.5087	1.554	1.131
3	2.54×10^{-4}	15.63	0.5087	1.289	1.175
4	6.35×10^{-5}	63.5	0.5087	0.358	1.326

The mass percentage of samples in experimentation were determined to be within the range of 1.18% to 1.30% for the four dilutions formed. As described in the ASTM method, further determination of the volume percentage of naphthalene in jet fuels can be determined within the utilization of the mass percentage value calculated.

Discussion of Volume Percentage of Naphthalene Calculations:

M: Mass percentage of Naphthalene, by mass
B: Relative Density of the total fuel (15 ℃ / 15 ℃)
C: Relative density of the naphthalenes (15 ℃ / 15 ℃) = 1.00

$$\text{Naphthalene, Volume \%} = M \times \left(\frac{B}{C}\right)$$

Figure 8: Formula for determination of the volume percentage of naphthalene in solution.

Further determination of volume percentage of naphthalene in jet fuel samples can be calculated utilizing the formula in Figure 8 which relates the calculated mass percentage of naphthalene, by mass solution with the relative densities of jet fuel samples and naphthalene in solution.

■ Conclusion

Shimadzu's UV-Vis 2600i demonstrates great versatility in the examination of di-aromatics in solution. Data analysis of samples revealed mass percentages of naphthalene between 1.1% to 1.3% in solution. Assessment of naphthalene contents in solution is simplified with Shimadzu's spectroscopic instrumentation, including characteristic peak identification required for data evaluation. Naphthalene detection is achieved through a user-friendly software, eliminating the need for complex configurations for sample scans, and proving highly effective for industry application.

■ References

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