

## 다이오드 레이저 비색 분광기를 이용한 Cetylpyridinium Chloride의 농도분석

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### Application of a Diode Laser Colorimetric Spectrometer to Determination of Cetylpyridinium Chloride

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#### Summary

In order to analyze the concentration of cetylpyridinium chloride(CPC), a widely used cationic surfactant, we developed a simple and compact spectrometer, which consisted of a diode laser and a photodiode detector. Preliminary results are described here on the performances of the system in terms of the stability of output intensity, sensitivity, and reproducibility. Data on the comparisons of the system with the conventional UV-VIS spectrometer are also given. With the instrument, the concentration of CPC between  $3 \times 10^{-5}$  M and  $1.1 \times 10^{-4}$  M are calibrated as a correlation coefficient of 0.9635. The results shown here indicate a potential for developing a portable spectrometer useful for analyzing concentrations of CPC.

#### 1. Introduction

Cetylpyridinium is classified as a cationic surfactant and is one of the very important surfactants that is widely used in industrial and pharmaceutical substances, especially in manufacturing of dermal ointments, drugs and cosmetics. The formation of ternary chelate compound of CPC with bromopyrogallol red(BPR) and strontium is accompanied by a marked increase in the absorbance and a bathochromic shift in the maximal absorption of the complex from 555 nm to 627.5 nm. On the basis of the color change of CPC from red to blue, the colorimetric quantification of CPC was achieved.(1)

The visible diode laser of 630-670 nm wavelength has

been recently and widely used in optical spectroscopy because the light source in the region has a long lifetime, power stability, low power consumption, small size, and low price. Even though output power of a diode laser is usually limited to 3-30 mW, is comparable to the power of a xenon arc radiation passing through the monochromator in a conventional UV /VIS spectrometer.(2) Therefore, a diode laser could replace the radiation source and a monochromator in the conventional UV/VIS system, and simplify the development of a practical and specific analytical instrument.(3-8)

Since the emitting wave-length is agreed with the absorption maximum of blue colored CPC, ternary chelate compound of CPC with BPR and strontium,

the developed system was applied to the analysis of CPC.

In this paper, we describe the structure of the compact and simplified spectrometer with a diode laser of 633-nm radiation, double beam system, and photodiode detector. And also evaluate its performances, comparing data of the developed system (Diode Laser-Double Beam Colorimetric System, DL-DBCS) with those of the UV/VIS spectrometer.

## 2. Experimental

### 2.1 Instrumentation

The system is depicted in Figure 1. This system features a diode laser, a double beam system, and a photodiode detector. The 633 nm diode laser (LDM 145/633/5, Imatronic Co., Ltd., USA) was used. The laser beam was focused by a convex lens (F.L.= 6 cm). The beam splitter separated a signal beam and a reference beam from the laser beam. A simple photodiode (Pin-6DP, UDT Sensors Inc., USA) was used for detection. The signal was amplified and sent to the RS232C port of a notebook-PC using A/D converting system(Home Made). In order to compare the results obtained from the conventional method, a UV/VIS spectrophotometer (UV-2101PC, Shimadzu, Japan) was used. The line profile of the diode laser was measured by using a conventional grating and a CCD detector(SD-1000, Ocean Optics, USA).

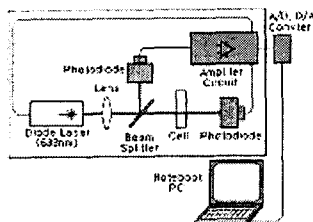


Figure 1. A schematic of the Diode Laser-Double Beam Colorimetric system (DL-DBCS).

### 2.2 Reagents and Procedure

Cetylpyridinium chloride, bromopyro-gallol red and strontium (II) were from Aldrich (Analytical grade) and used without further purification. A  $1 \times 10^{-2}$  M cetylpyridinium chloride stock solution was prepared by dissolving 895.0mg of cetylpyridinium chloride in distilled water. The required cetyl-pyridinium chloride standard solution was prepared daily by dilution of the stock solution. A strontium (II), bromopyrogallol red and buffer solution were prepared respectively  $1 \times 10^{-2}$  M,  $1 \times 10^{-3}$  M and  $1 \times 10^{-2}$  M. In order to obtain a calibration curve, 4ml of each standard solution, 0.4ml of strontium solution, 0.4ml of bromopyrogallol red, and 0.2ml of buffer solution were vigorously mixed. The blue color formation of ternary chelate compound was completed in 20 minutes.

## 3. Results and Discussion

### 3.1 Radiation Profiles of the Diode Laser

In Figure 2, the solid line is a radiation profile of the diode laser between 450 nm and 750 nm wavelength obtained by conventional grating and CCD detector. The dotted line is the absorption spectrum of ternary chelate compound measured by a conventional UV/VIS spectrophotometer.

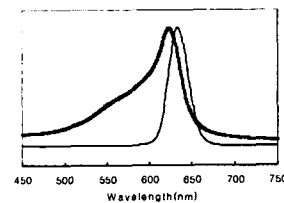


Figure 2. A radiation profile of the 633nm visible diode laser (-) and absorption spectrum of ternary chelate compound of CPC(\*) between the wavelengths of 450 nm and 750 nm.

The solid line forms a Gaussian shape whose peak is located at 633 nm and whose width of the half maximum is 29 nm. The wavelength at the peak of the diode laser is well agreed. The narrow bandwidth is

included in the broad absorption spectrum of colored ternary chelate compound. These characteristics suggest that the diode laser can be applied to molecular spectroscopy for detecting ternary chelate compound.

### 3.2 Stability of the DL-DPCS

In Figure 3, the solid line is the trace of absorbance of the DL-DPCS according to time, and the dashed line is that of the UV/VIS spectrometer when the sample cells have the standard solution. In the conventional system, the base line is stable and located at zero absorbance. On the other hand, in the DL-DPCS, the base line is slightly unstable and oscillates. It is believed that this slight unstableness probably occurs by a change of hole-electron pairs according to temperature changes in the diode laser. The noise, however, is smaller in the DL-DPCS than in the conventional system and the oscillation is within the noise level of the conventional system. Consequently, the base absorbance by the system is expected to have no effect on measuring the absorption of ternary chelate compound.

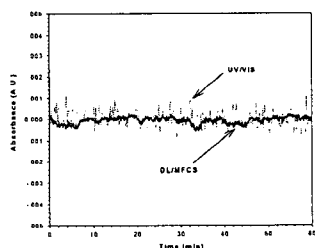


Figure 3. Stability comparison between DL-DPCS(-) and conventional UV/VIS (--)

### 3.3 Calibration and Evaluation of the Instruments

Figure 4 shows the calibration curves of ternary chelate compound for conventional UV/VIS and the DL-DPCS. In the DL-DPCS, with the increment of the concentration of cetylpyridinium chloride from  $3.1 \times 10^{-5}$  M to  $1.1 \times 10^{-4}$  M, the absorbance increases linearly with a slope of 7785.2 AU/M and intercept of

$1.153 \times 10^{-1}$ , and a correlation coefficient of 0.9635. While, for the conventional UV/VIS spectrophotometer, slope, intercept, and correlation coefficient is 16219.6 AU/M,  $1.539 \times 10^{-1}$ , and 0.9906 respectively.

From these results, we anticipate that the developed system has enough possibility to be utilized in practice.

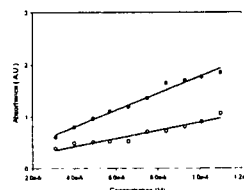


Figure 4. Calibration curve for CPC using DL-DPCS (○) and conventional UV/VIS (□).

## 4. Conclusions

In spite of its simple and inexpensive structure, the Diode Laser-Double Beam Colorimetric System reveals the good performances to determine the cetylpyridinium. This instrument can also be introduced for the detection of other chemical compounds if the blue color develops in the solution of the chemical reaction. In addition, other chemical species could be detected by the colorimetry, if the laser diode was replaced by other laser diode whose radiation wavelength matches up to the color of the compounds. These studies are in progress in our laboratory.

## 5. References

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