USING LEGO MINDSTORMS NXT™ ROBOTICS KITS AS A SPECTROPHOTOMETRIC INSTRUMENT

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Abstract -High-end spectrophotometric analytical instruments are typically employed in academic institutions and industrial research laboratories and are rarely available for experimenters or younger students. An affordable high-tech robotic product manufactured by Lego may be employed as a single-beam monochromatic light source, detector and display to demonstrate and investigate the Beer-Lambert law using solutions containing chromophores that absorb light in the 600 nm - 660 nm range. Using the materials shown in this work, users will gain an understanding of the measurement of optical properties of solutions, and basic properties of semiconductor photonic devices. Some semiconductor theory is essential to understand the photonic devices employed in this work in addition to an understanding of basic analytical chemistry The majority of this work addresses the relationship between concentration and absorbance.

Index Terms - Absorbance, Chromophores, Microcontroller, Reflectance, Robotics, Solution, Spectroscopy, Spectrophotometric Instrumentation.

I. INTRODUCTION

Microcontrollers are ubiquitous and are found in practically every commercial product from toasters to televisions. Low-end 4-bit microcontrollers are commonly employed in appliances requiring simple timing control and are considered where cost saving is imperative. High-end 8-bit, 16-bit and 32-bit devices containing internal analog-to-digital (A/D) converters are found in most instrumentation applications where cost sensitivity is not of concern. Microcontroller technology has matured and proliferated such that peripheral functions, such as LCD drivers, internal A/D, high-resolution timers and electrically erasable programmable read only memory (EEPROM), can be included in the end product for marginal cost.

Robotic technology has enjoyed significant recognition as an industrial tool and an extension of human function. When coupled with advanced software algorithms that employ fuzzy logic and control theory, predictive machine behaviors may be emulated. Predictive behaviors as such may be employed as guidance control where real-time maneuvering may be performed (1, 2). Advanced optical sensing and pattern recognition in robotic systems has been employed to emulate human motion and mirror image cognition (3). Simple gaming theory applied to fuzzy logic control using optical sensors to detect color objects has also been of interest (4). Advanced robotic applications include possible recognition and discrimination of threats to human and animal life (5). Common to these applications are the necessity for high-end computing power that require high speed and advanced numerical processing capability. Basic signal recognition and simple motion control can be emulated with low-end microcontrollers and robotic systems, however.

An example of low-end robotic technology has been the Mindstorms™ and Mindstorms NXT™ kits from Lego (*6*). The objective of the product is to teach basic robotic principles that integrate mechanics with sensors and also teaches visual programming skills using drag and drop menus to build logic that may be downloaded to the kit's embedded EEPROM. The NXT incorporates an ST Microelectronics ARM-7 32-bit microcontroller operating at a 48 MHz internal clock speed. The kit also contains the necessary hardware ports to interface with real-time peripheral sensors, specifically, acoustic transducers, tactile switches, accelerometers and optical transducers.

In this work, the Lego 9844 light sensor is employed. The sensor contains a red LED to generate an optical signal in the 632 nm ± 3 nm region. The sensor contains an SFH309-4 phototransistor acting as the light detector. The sensor is typically configured to measure the reflected light from the internal red LED but may be configured in firmware to measure ambient light. Because the products are considered open-source, schematics for the NXT and the sensors are available online (*7,8*). The code is also open-source as most of the functionality was derived from National Instruments LabVIEW™ graphical user interfaces (GUI) programming (*9*).

The NXT contains a low-resolution LCD capable of displaying some graphics and text. In this work, the built-in optical reflectance measurement function contained in firmware is employed to measure optical transmittance. The display is updated in real time in one-second intervals. The reflectance function is accessed using a simple menu by pressing a series of keystrokes on the device's front panel. To maintain simplicity and ease of operation, the built-in reflectance function is used; some optional programming may be performed to convert the reflectance to absorbance. Again, in the interest of simplicity, the real-time reflectance measurements may be logged on paper and subsequently converted to absorbance using Excel™ or Origin Pro™ software.

The materials used in this work are shown in Figure 1. The Mindstorms NXT™, 9844 light sensor, six solution samples, one blank, ringstand and clamp are shown. A silvered mirror and 1 cm cuvette are required but not shown in the figure.

Figure 1. The Lego Mindstorms NXT™, 9844 optical sensor, ringstand, clamp and solutions used in the experiment are shown. A silvered mirror and 1 cm glass cuvette are not shown.

The silvered mirror was prepared using vapor deposition onto a glass microscope slide for previous optical experiments; any polished reflective surfaces will reflect the optical signal when placed behind the cuvette, however. Figure 1 shows the system during power-up state with the LCD and sensor active. The active region of the light sensor is shown in Figure 2. The red LED emitter appears as the bottom optical device; the phototransistor (detector) appears at the top. A molded planar surface bisects the two optical devices to provide some optical isolation. The image at the right of Figure 2 shows the source in the power-up mode. The NXT™ firmware allows the detector to also work independently of the LED. One of the fundamental menu options toggles the LED state ON / OFF allowing the instrument to measure ambient light intensity.

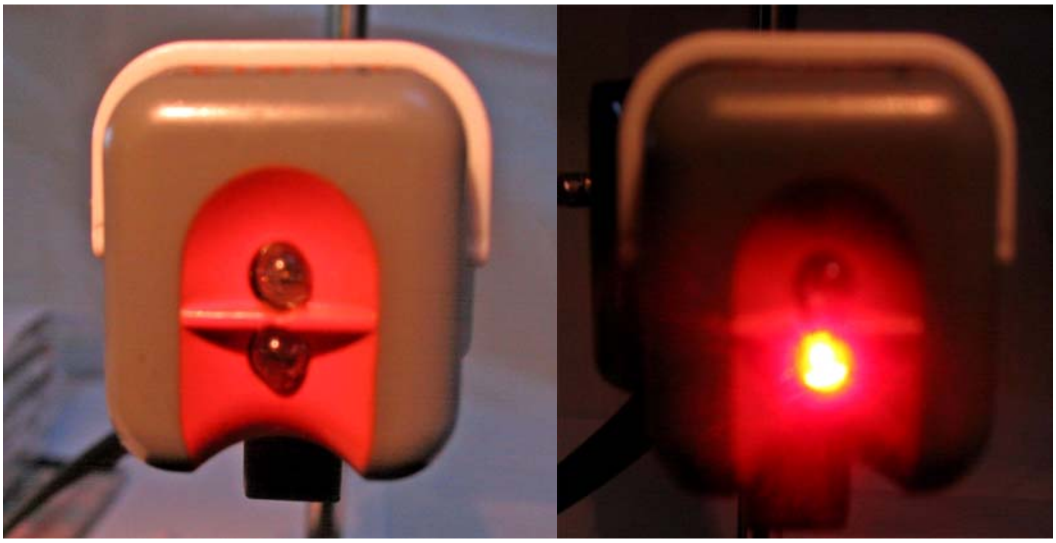

Figure 2. The 9844 optical sensor contains an SFH309-4 phototransistor (upper optoelectronic device) and red LED (bottom device), both shown in the left-hand picture. A molded planar surface provides some optical isolation between the source and detector.

Commercial spectrophotometers typically employ an incandescent light source and a monochromator consisting of a prism or diffraction grating to select the desired wavelength. The emitted beam is passed through a cuvette containing the analyte; the optical signal transmitted through the analyte is converted to a current using a photodetector and recorded. The optical path length is typically 1 cm using a standard cuvette. Scattering effects in dilute solutions are usually negligible. Beer’s law states that the absorbance of the incident light is linearly related to three factors (*10, 11*):

$$A = abc \qquad \text{(Eq. 1)}$$

where a is the molar absorptivity of the analyte, b is the optical path length and c is the concentration of the analyte. Absorbance is related the ratio of transmitted to incident light intensity by the following relation:

$$A = \log(1/T) \qquad \text{(Eq. 2)}$$

where the transmittance T is:

$$T = I/I_0 \qquad \text{(Eq. 3)}$$

where I is the transmitted intensity and I_0 is the incident intensity. Absorbance may also be described using:

$$\mathrm{A} = 2 - \log(\%\mathrm{T}) \qquad \text{(Eq. 4)}$$

A substance will absorb white light when it is either transmitted or reflected through it. Chromophores in the analyte make this light absorption possible. The eye does not see the wavelengths that are absorbed by a sample. Rather, the complimentary color of the absorbed wavelength is observed (12). An absorption spectrum will indicate how absorption occurs with a continuous spectrum of incident light. At the highest peaks of absorbance, it is possible to estimate that the complimentary color will appear in a substance. Prediction of the absorbed colors may be performed by employing a color wheel and observing the compliment containing the incident color or colors.

Color can also be understood by the electronic transitions that take place and the molecular level. A photon will interact with a molecule when it comes into contact with a light source. The molecule will be promoted into an excited state. This alters the distribution of electrons, or molecular orbital. An electronic transition occurs because the excited state will move from one molecular orbital to another. This movement causes either an increase or decrease in energy. These transitions occur at allowed wavelengths that will only be observed as color if they are in the visible spectrum of light.

Commercial spectrophotometers employ the shortest optical path length from the source, through the cuvette, and to the photodetector (Figure 3a). Most commercial spectrophotometers are dual-beam instruments that employ a second optical path that measures the properties of a blank solution. The absorbance signals measured from the blank are subtracted in software. Using the 9844 optical sensor without modification requires that the source and detector are inherently adjacent and will rely on a signal reflected from the mirrored surface behind the cuvette. This, in effect, doubles the optical path length and also increases the divergence of the light beam (Figure 3b). The net result is the I/I_0 signal will be at least 50% of that expected with an in-line source-detector path.

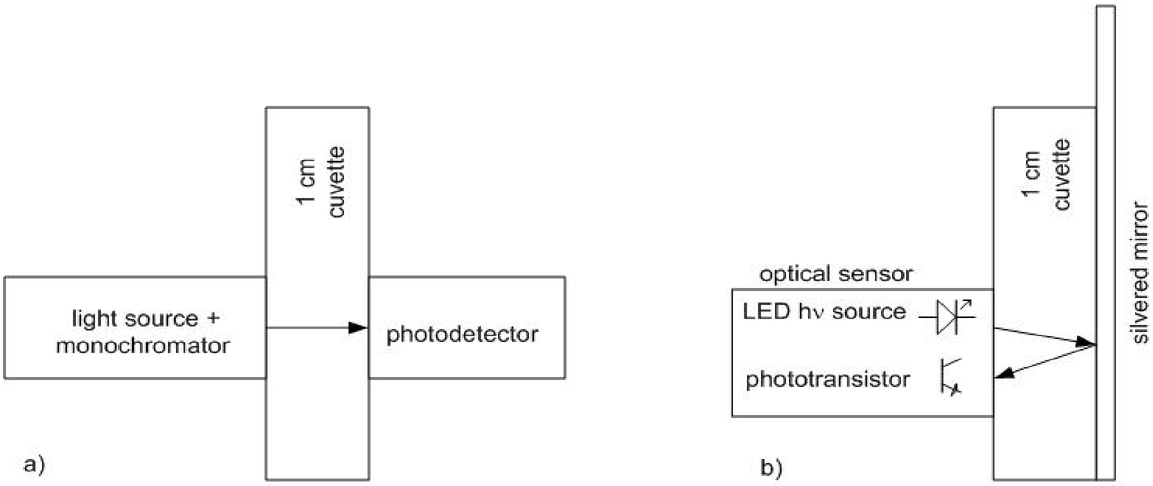

Figure 3. Commercial spectrophotometric instruments employ a single-beam or dual-beam optical system that place the sample cuvette in line with the source and detector (a). The experimental system employed in this work utilizes the combined source (LED) and phototransistor (detector) in a single package. The optical path through the analyte / cuvette rely on reflection from a mirrored surface placed behind the cuvette (b).

II. EXPERIMENTAL

A standard solution was prepared using McCormick green food color with 0.500 mL dye in 100 mL of double deionized H_2O. The exact concentration of chromophores in the commercial food color is unknown; hence all references are made to the prepared standard solution of 0.500% (V/V). A series of five 2:1 serial dilutions were performed (Figure 4).

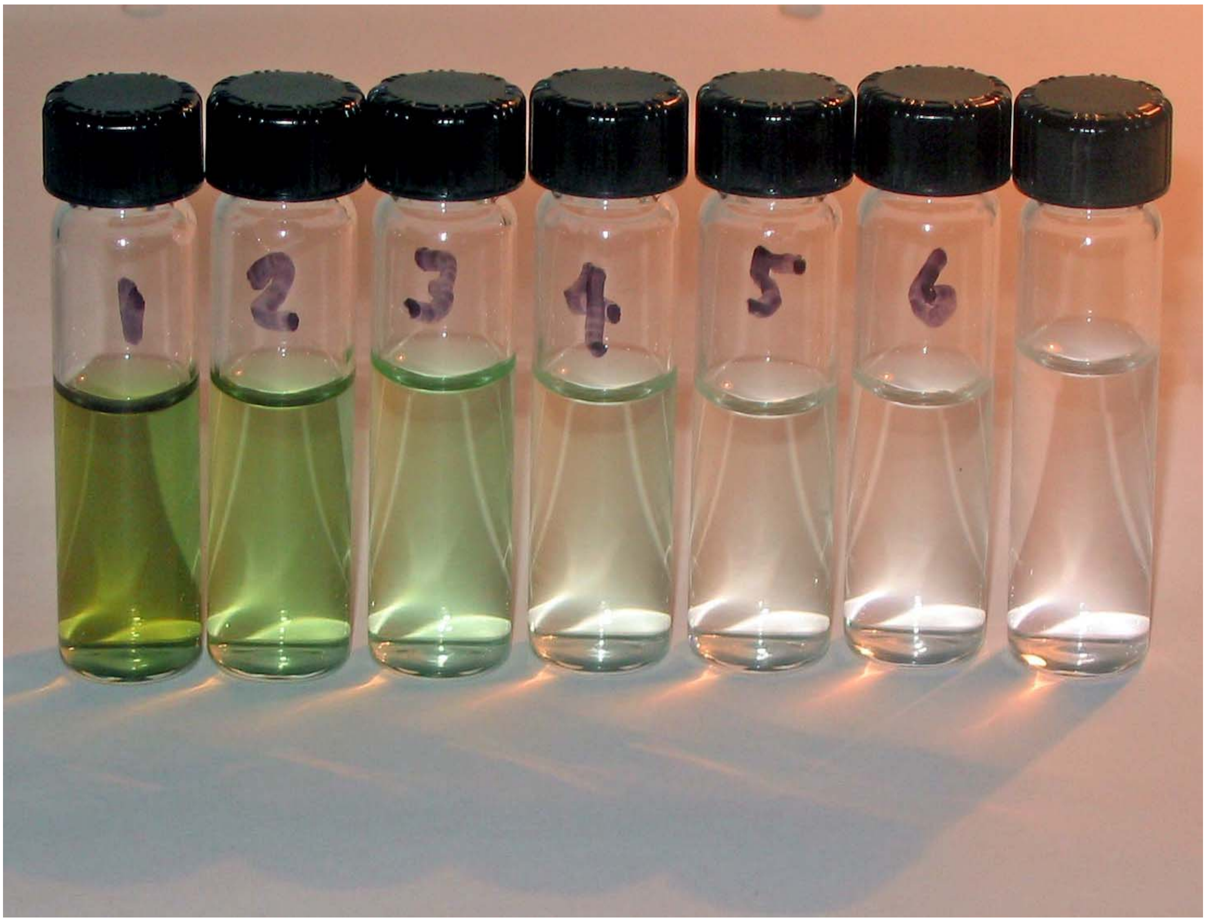

Figure 4. A standard 0.500% (V/V) solution was prepared using McCormick green food color (vial 1). Successive 2:1 serial dilutions were made (vials 2-6). The unlabeled vial contains the double-deionized H_2O blank

These solutions have the inherent advantage that the absorbance peaks are optimized with the peak wavelength of the 9844 emitter (Figure 5). Another advantage to using the commercial food color is that it is safe, unlike working with inorganic salts that pose a level of toxicity if handled incorrectly. Inspection of the family of transmittance curves shown in Figure 5 indicates the presence of two chromophore species in the green solution. The sharp absorbance peak at 630 nm indicates the presence of a green chromophore while the broad absorbance peak at 415 nm indicates the presence of yellow chromophores. Closer inspection shows that a minor absorbance peak at 525 nm indicating the presence of small amounts of blue chromophores. Again, note that the dilution factor is doubled for each concentration. The transmittance curves were generated using a Hitachi U-2000 spectrophotometer.

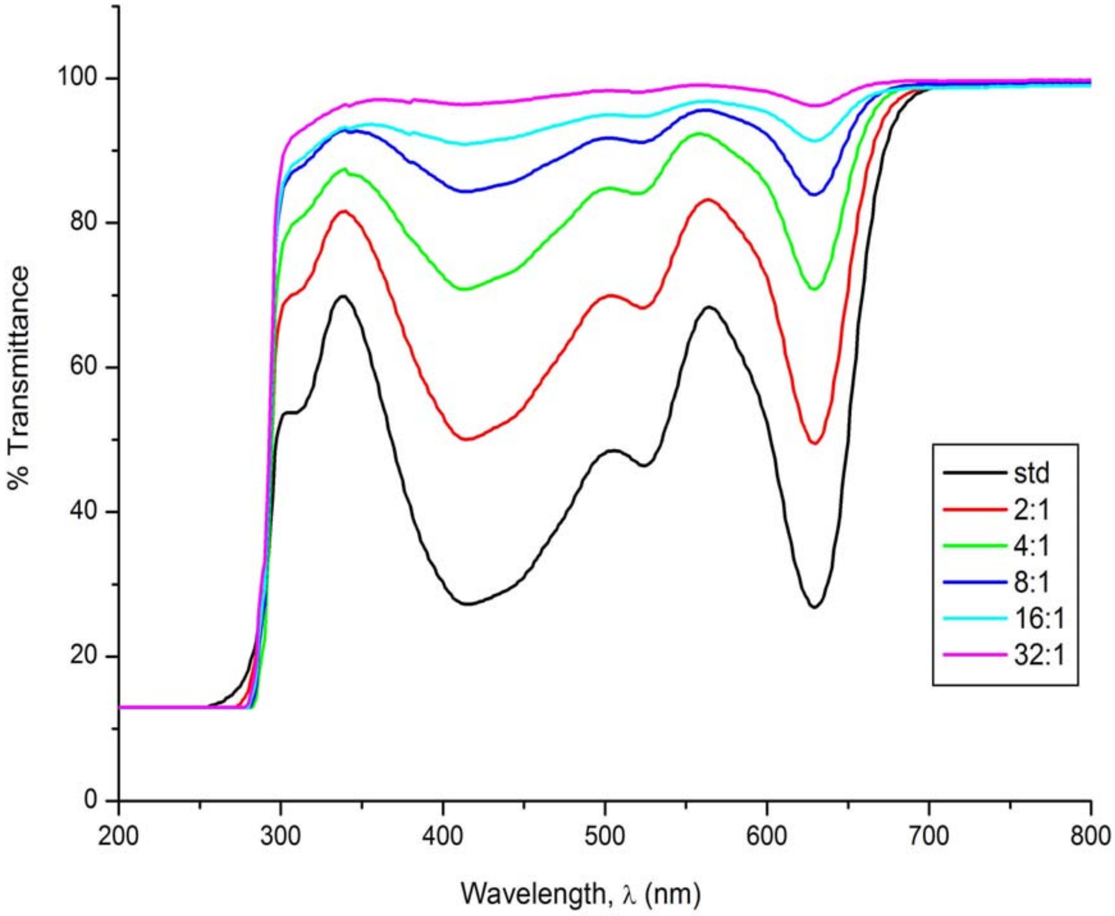

Figure 5. Transmittance data obtained from a series of binary dilutions of green food color solution using a Hitachi U-2000 spectrophotometer. Two prominent absorbance peaks are observed at 630 nm and 415 nm indicating the presence green and yellow chromophores, respectively. A minor absorbance peak at 525 nm indicates a small quantity of blue chromophores present in solution.

Transmittance data were obtained for the six solutions and blank using the NXT™ system. Absorbance was calculated using Equation 4 and subsequently normalized by subtracting the infinite dilution value from each (Table 1). Figure 6 shows the resultant corrected absorbance from the Mindstorms™ photometer compared to the Hitachi measurement system. There is a small degree of nonlinearity in the absorbance plots. This may be attributed to the longer path length, beam divergence and scattering as expected with solutions of higher concentrations. This effect is more pronounced in the Mindstorms™ data.

Table 1. Transmittance and absorbance data obtained using the 9844 sensor.

Dilution	STD	2:1	4:1	8:1	16:1	32:1	inf
% Transmittance	46	60	69	75	78	80	82
Absorbance	0.569	0.420	0.319	0.268	0.229	0.208	0.187
Corrected Absorbance	0.251	0.138	0.075	0.039	0.022	0.011	0.000

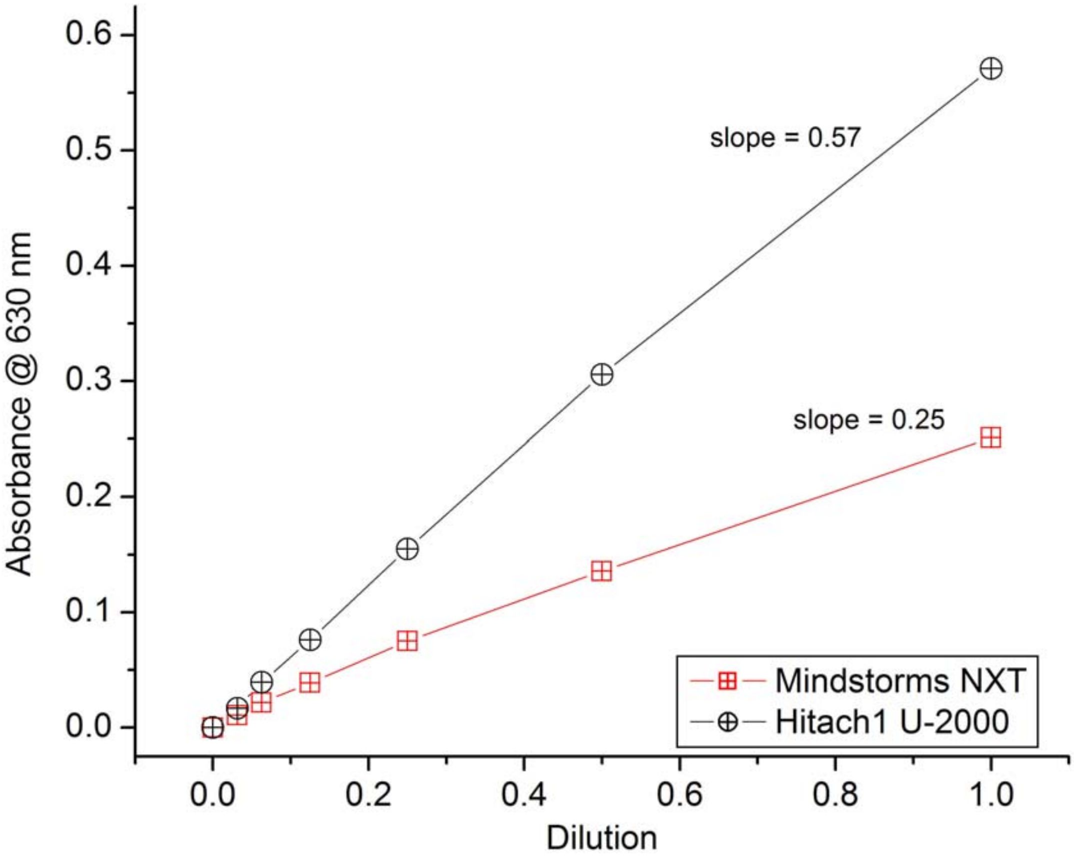

Figure 6. Absorbance plot derived from corrected data in Table 1 and from transmittance data measured with Hitachi U-2000 spectrophotometer. The Hitachi transmittance data was converted to absorbance using Equation 4.

Note the difference in the absorbance slopes. This difference is attributed to the light leakage from the source to detector in the 9844 sensor as the devices are located adjacent in the same enclosure. A molded planar surface between the two optical devices shown in Figure 2 provides some isolation, however some backscattering of the optical signal decreases the sensitivity to the properties of the solution. It appears that this effect is tolerable so that the basic principles of Beer's law may be demonstrated, nevertheless.

III. CONCLUDING COMMENTS

We have demonstrated that the sensors and signal processing tools available in the Lego Mindstorms™ products are a viable resource for introductory chemistry labs at the high school or junior college level. The work also serves as a basis for further experimentation for other applications in the laboratory. Here we have addressed the ability of the product to measure absorbance of green chromophores. It is suggested that minor modifications to the 9844 sensors be performed to replace the red LED with devices that emit monochromatic light of other wavelengths. Again, considering that the schematics are available online, further experimentation may be made to adjust the gain and offset of the phototransistor output by changing resistor values. It is also possible to implement an in-line cell that utilizes a shorter optical path length by removing the LED from the sensor package and mounting it externally precisely opposite the phototransistor.

If desired, users could also prepare individual silvered reflective surfaces as part of this experiment or an adjunct exercise. The procedures for preparing silvered surfaces either chemically or by electroplating are relatively simple and can be used to demonstrate additional chemical principles, including oxidation-reduction reactions and electrochemistry (13).

Our objective for future work is to develop intelligent technology based upon optical sensing and impedance spectroscopy employed as remote robotic-based electronic olfaction systems to detect atmospheric-based organic vapors and contaminants in liquid or soil samples. These technologies have possibilities for military and space applications.

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