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An instrument for instant identification of chromatic changes in chemical reactions

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Colour change in a chemical is an indication of one of several causes. The reaction of the chemical occurs with the addition of another organic or inorganic substance. To monitor a reaction as it takes place, during the transition of its molecular structural properties, colour change is a useful criterion. In industrial manufacture of chemicals through their formation with many a combination and technique, to arrive at the needed composition, colour change is a very useful criterion. An instrument that can detect instantly and record the changes in the colour of the reacting substance has been developed, which uses a Provotech sensor. Using an embedded controller, and an exhaustive software to sense the colour, it can report the parameters quantitatively from instant to instant; it is a very compact and simple one to use in the laboratories or in production. The artificially intelligent program can sense and report colours by names in addition to the more detailed quantitative colour space parameters. The controller could also initiate action to time a reaction to occur, to stop a reaction at the intended level by the sensing of the changes in hue, say from 640 nm to 650 nm. Though a simple and economical instrument, it provides useful colour value information during the transition phase of any reaction and reports the data to a computer in addition to a display on LCD of the hue, saturation and colour name, such as reddish purple.

Keywords: Provotec sensor, embedded controller, C.I.E. chromaticity diagram, colour space, FTIR.

Introduction

A chemical change is due to the combination of one or more substances by reaction and synthesis or decomposition to form more substances. They are generally irreversible except by further chemical reactions. There are three types of chemical changes namely organic, inorganic and biomedical changes. Organic compounds will contain a carbon atom (and often a hydrogen atom, to form hydrocarbons), while almost all inorganic compounds may not contain either of those two atoms. Few inorganic compounds containing carbon are carbon monoxide, carbon dioxide, carbonates, cyanides, cyanates, carbides and thiocyanates. In a chemical reaction, a chemical change must occur which is generally observed with physical changes like precipitation, heat production, color change etc. In a physical change, there is basically a change of state of the substance but in the case of a chemical change mostly a new substance is formed in which either energy is given off or absorbed. Thus, chemical changes are accompanied by certain physical changes. A reaction can take place between two atoms or ions or molecules and they form a new bond and no atom is destroyed or created but a new product is formed from reactants. Thermally induced molecular reactions are another. Reactions by photo excitation through irradiation even with solar light are well known. Combined with organics substances, colour changes are found in very many more substances, leuco dyes for instance. Chemicals are used throughout industry to make a wide variety of consumer goods, and are also indispensable in diverse industries such as food, agriculture, life sciences, and many service industries.

Many reactions in inorganic chemistry involve the colour changes associated with them. For example, cuprous mercury iodide Cu_2HgI_4 changes colour due to phase change at about 67°C (dark brown to bright red). Silver mercury iodide changes colour from yellow to orange, mercury iodide from red alpha to pale yellow. Combined with organics substances, colour changes are found in very many more substances. Oxides of chromium(III), aluminium(III) and vanadium provide scope of colour change studies.

The thermochromatic liquid crystals are used to prepare *“the mood ring”.* On the other hand, the leuco dyes could be applied on the papers, polymers and inks. Leuco dyes is popular to create magic papers and inks to write *secret* messages. However, the most polar use of leuco dyes is on the polymers to create magic t-shirts and *color changing mugs.*

In nano chemical particles, reactions occur too rapidly and the transition phase can be very difficult to observe except with very sophisticated set up of instruments.

Better methods of sensing reactions exist, such as instruments like differential scanning colorimeter, Fourier Transform infra-red spectrophotometer, UV spectrometer, flash photolysis analyser, to name but a few.

Detecting chemical changes by colour:

Alchemists try to turn elements and other substances into gold. Modern scientists have achieved this feat using particle accelerators and nuclear reactions; it is to make a chemical *appear* to turn into gold. Another fascinating color change reaction is the Water-Wine-Milk-Beer Color Change Reaction.

Popular within research and manufacturing environments, high performance, precise color measurement solutions help organizations formulate, evaluate, and control color to meet product quality and operational goals more efficiently. To see which solution best fits the application and operational needs, selection is made among colorimeters, spectrophotometers, gloss meters and also the software. Instrumental color measurement moves beyond the limits of human perception and vocabulary and allows us to capture color information as objective data, creating *a common language of color* that is essential for communication within and between industries around the world. The two most advanced color measurement instrument types are colorimeters and spectrophotometers, both of which use sophisticated technologies to accurately and precisely quantify and define color. While closely related, these instruments have unique qualities that may make one more suitable than the other for a particular type of measurement.

Colorimeters are extraordinarily accurate for straightforward color measurement and ideally suited for determination of color difference, fastness, and strength as well as routine comparisons of similar colors. As such, they can be invaluable for color quality control and are primarily used in the production and inspection phases of manufacturing. Though colorimeters can produce highly accurate color measurements, they are *not able to identify metamerism* or colorant strength, are not ideally suited for color formulation, and cannot be used under variable illuminant/observer conditions.

A spectrophotometer[1] is an instrument designed for physical sample analysis via full spectrum color measurement. By providing wavelength-by-wavelength spectral analysis of a sample's reflectance, absorbance, or transmittance properties, it produces precise data beyond that observable by the human eye. Full spectrum analysis also provides for greater specificity, potentially identifying color differences missed by colorimeters. Type of data required, instrument geometry, precision and accuracy, light source, rapidity of measurement, ease of use, robustness, software interface and product quality determines the instrument to be used.

Importance in the lab and chemical industries:

Laboratory titration of chemicals relies mostly on colour indication. From glycol acids to aromatic solvents and chlorinated paraffin, liquid chemicals can be opaque, translucent paraffin, liquid chemicals can be opaque, translucent or transparent, so requires different instrumentation techniques for successful color measurement. Petrochemicals include olefins such as ethylene and propylene, benzene, toluene and xylene. They are the building blocks for a wide range of materials such as solvents, adhesives, plastics resins, fibers, elastomers, lubricants and gels.

From polymers to plastics, fertilizers to pharmaceuticals and petrochemicals, manufacturers rely on instruments to provide solutions to ensure quality and consistency of their product. Quantifying color to visual perception through criticals metrics and indices such as APHA/Haze, Plt-Co, Whiteness, Yellowness, Gardner, Saybolt and Haze are useful to check color consistency and quality across supply chains.

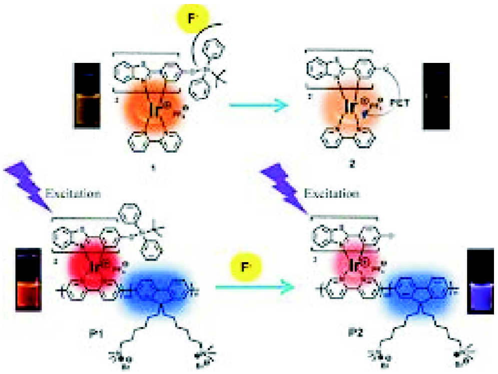

Fig. 1. An insight into the changes in colour during chemical reactions.

Opaque liquids are impenetrable by light and are best measured using reflectance geometry. Translucent liquids allow light to pass through, but onlyu diffusely, so that objects on the other side cannot be clearly distinguished. Both reflective and transmittance measurement modes may work well depending on the translucency of the sample.

Rapid chromatic detection of bacteria is yet another colour sensing application[2,3]. Colour changes in skin are also reported to be of good diagnostic value[4].

Control action based on a critical colour change is often needed in synthesing chemicals. An automatic colour sensing with alarm annunciation is also required in many synthesis applications.

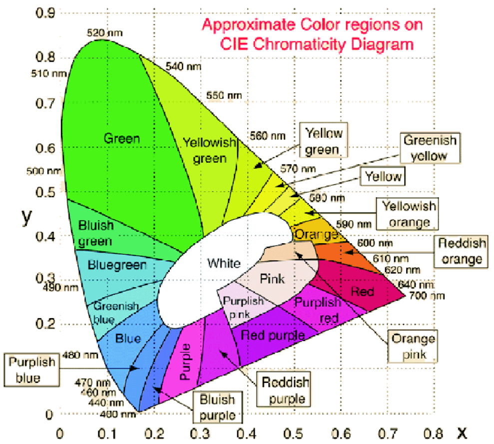

Fig. 2. Chromaticity chart with x and y being the red and green co-ordinates.

Description of the colour measurement instrument:

Herein is described an unit useful for instantly identifying the changes in colour, with reporting on changes for annunciation and control action. It consists of a colour sensing sensor unit and an AT Mega 328 microcontroller. The colour sensor is provided with its 5 V supply and signals from the photo diodes are in the range of 0 to 0.5 V. These values are read by ADC in a microcontroller. The AT Mega 328 is a fairly powerful chip with ADC channels and with a crystal of 16 MHz has a processing speed of 16 MIP (Million Instruction per Second). The instrument is constructed so as to provide an instant display of the several colours classified in 23 categories, based on the colors from the chromaticity chart. Its software can report hue in nm, saturation or purity of the colour and lightness value.

The sensor is a Provotech make[5] and is interfaced to the AVR ATMEGA 328 chip via the ADC pins. This very chip also is used in the well known Aurduino microcontroller kit. Here, the Arduino board is not used, but the circuit just uses the chip separately. There are several ADC input pins in this chip. So, three of them are connected to read the three signals from the Provotech Sensor. They are the Analog input pins for channels red, green and blue from the sensor. The ADC in the device has provision for reference voltage values of V_{CC}, any voltage connected to the V_{ref} pin or the internal 1.1 V reference. The sensor outputs are low voltage values, within 0–0.5 V. So, the ADC is programmed to have an internal reference of 1.1 V from within the chip, so that the signals which are within 1 V only can be got as numbers in the range 0–255. This means, we do not need any external amplifier for the signals, since it is difficult to construct a simple direct coupled amplifier without drift. This is the special advantage of using this AT Mega 328 chip.

The circuit is also interfaced to a two row character LCD display. As is usual with such LCDs, there are the following connecting lines to the microcontroller:

RS (Register select) pin 4 of LCD

R/W (Read or Write) pin 5 of LCD

E (Enable) pin 6 of LCD

Pin 1 is ground; pin 2 of LCD unit is the 5 V supply to be applied. The pin 3 is connected to a preset resistor of 10 K to adjust the voltage between 0 and 5 V for varying the contrast of the characters shown on the LCD display module.

The data comprises of four wire connection to the pins D4 to D7 of the LCD (11-14). Here, a four wire data connection rather than the 8 wire data connection is used. The pin 15 is for backlight of the LCD and pin 16 is grounded.

An illustration of a laboratory chemical reaction undergo-

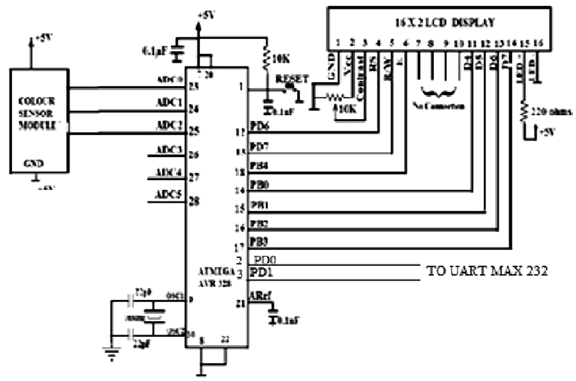

Fig. 3. Circuit diagram of the color identification and annunciation unit.

ing colour transitions is shown in the Figs. 5 (a to c).

The response curve can be plotted in terms of the change in hue with time in the X axis, as shown in Fig. 4.

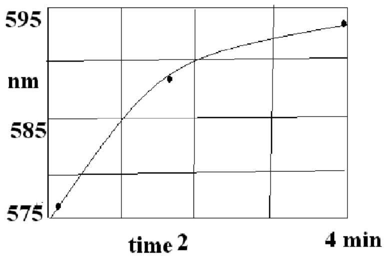

Fig. 4. Response of reaction by colour.

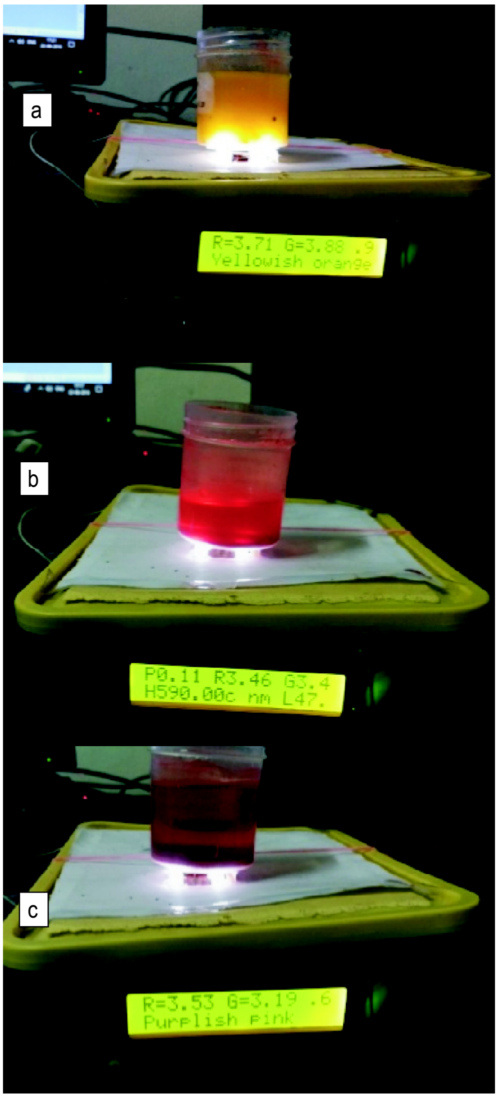

Fig. 5. (a to c) Photograph showing a lab chemical colour change from 570 nm to 590 nm – from yellowish orange to pink and purplish pink.

This software (which is written and compiled in BASIC language) is very helpful for developing the project even though the instructions are extensive. The hex file for programming the AT Mega 328P chip is also generated by the AVR simulator IDE by Oshon.com.

Conclusion

The instrument sends data on colour to the laptop through the serial port. The computer program will initiate an annunciation through beep sound or control to stop a reaction at the predetermined point by heat control or solvent valve control.

The data with respect to time of reaction can be plotted to show the response of the reaction via the colour change. Since data rate is fast enough, it can provide a good response indication even for fast reactions of the order of a hundred millisecond.

The instrument is capable of interpolating the color with in between Hues other than listed in the chromaticity chart, so it gives immense chance to measure even the minute change in color which is visually the same by using this instrument.

This unit could be further enhanced with a speech processor such as the aPR33A[8] to announce the hue/colour in addition to indication.

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