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A do-it-yourself Czerny–Turner spectrometer: atomic emission, absorption, reflection and fluorescence spectroscopy in natural sciences

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Abstract

Spectrometers play a decisive role in the education of A-level and/or under-graduate students in the field of natural sciences. They are capable to demonstrate atomic emission, transmission, reflection and fluorescence spectra, but can be used for wavelength filtering, as well. Here, we present a do-it-yourself spectrometer setup based on a Czerny–Turner design that (a) can be used for all measurement types with one and the same setup and (b) is capable to spectrally resolve atomic emission lines. We use LEGO® bricks for the optomechanical construction and combine it with affordable, but high-quality optical components and linear array based on a charge-coupled device (CCD). A modular design is implemented and allows for a quick

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change between the various measurement techniques, but also fosters the technological understanding of the underlying systems' optical design.

Keywords: UV–VIS spectroscopy, Do-it-Yourself, undergraduate, A-level, natural sciences, high resolution, modular

1. Introduction

Optical spectroscopy is an indispensable topic in scientific education for A-level and undergraduate students. On the one hand, the quantum theoretical principles of light–matter-interaction [1] can be experienced by means of atom line emission and absorption. On the other hand, a proper knowledge about the information that can be derived from the spectra of molecules and solid states [2] can be learned and is a mandatory prerequisite for starting-up in life sciences, physics, chemistry and many further research fields including cross- and interdisciplinary activities.

The pedagogical benefit of teaching the principles of modern spectroscopy by utilizing simple and modular photometers or spectral photometers has been reported, before [3–5]. Accordingly, a multitude of hands-on-experiments can be found in literature, most of them as do-it-yourself (DIY) setups with light-emitting diodes (LEDs) at low and moderate costs [3–19]. Some of the setups use digital or cell phone cameras for spectral detection [3, 5–7, 10, 11, 15, 18–21]. Most of them are developed for a specific application and measurement technique. The major weakness of these setups, however, is their limited spectral resolution. It limits the amount of information that can be derived from absorption and/or emission lines and may prevent first research experiences of students. Moreover, there is a risk that the basic principles of optical spectroscopy may remain unexplored, i.e. the pedagogical benefit may not occur.

We here introduce a DIY optical setup that (a) addresses the aspect of high-resolution spectroscopy, (b) can be applied for studies in different spectral windows at different spectral resolutions and (c) can be used either as atomic line emission, absorption, reflection or fluorescence spectrometer with one and the same system. Remarkably, the setup still is by about a factor of ten less expensive compared with commercial spectrometers of equivalent specifications and can be operated without in-depth instruction and preparation. It is thus very well suited for educational purposes.

2. Basic optical design in the context of teaching

The features of our system (cf figure 1(a)) are achieved by an optical design based on a Czerny–Turner (C–T) spectrograph [22], which is distinguished by self-correction of optical imaging errors. In addition, only a few optical components are required: a set of confocal mirrors (CM1, CM2), a reflective diffraction grating (RG) and an entrance slit (ES). Detection is realized by a CCD line-array or a projection screen. An LED serves as light source (LS) for transmission, reflection and fluorescent measurements (cf figures 1(a)–(d)).

The optical design of the C–T spectrograph may be the topic of a first teaching unit in spectroscopy. Following the light path, topics of fundamental optics are revisited: light passing the entrance slit ES (→ *diffraction at a single slit*) is collimated via the first confocal mirror CM1 (→ *lens equations*) onto a reflective diffraction grating RG (→ *Bragg condition of gratings*). The angular distribution of the diffracted light represents the spectral components of the incident light (→ *dispersion of light*), is collected by the second confocal mirror CM2 and finally projected into the image plane (→ *imaging optics*). Here, the spectral components are spatially separated from each other (→ *spectral resolution*), so that the signal intensity as a function of photon energy (→ *spectrum*), can be inspected by eye using a projection screen or electronically using a linear sensor array (CCD). Demand lessons may focus on the beam paths of the two confocal mirrors that are mirror-symmetric to each other in order to correct for optical errors (in particular for astigmatism related with the small tilt in the respective beam paths). A second teaching lesson may address the relation between spectral resolution and parameters of the

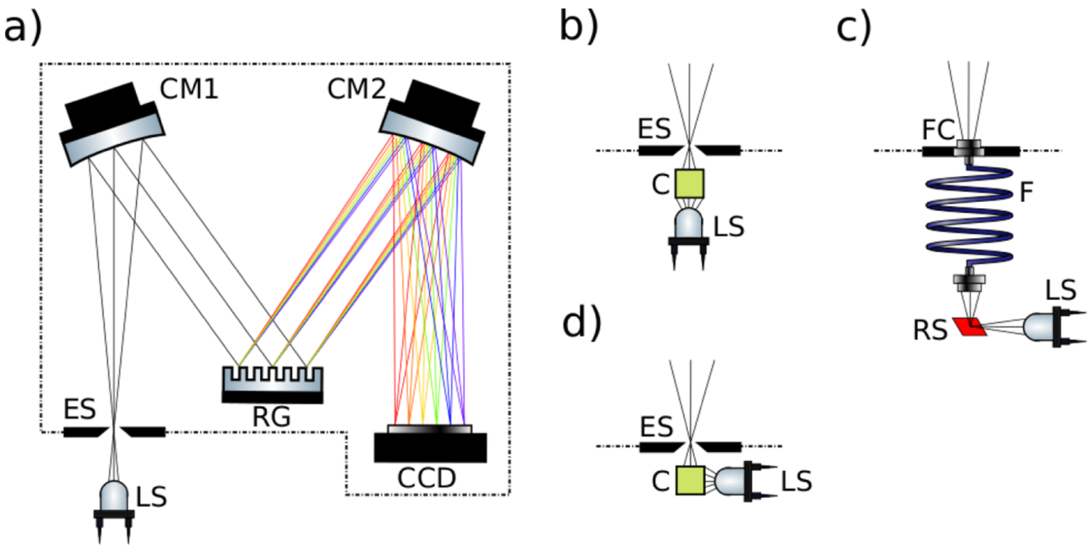

Figure 1. (a) Scheme of the DIY Czerny–Turner spectrograph for atomic emission spectroscopy: LS: light source (e.g. mercury vapour lamp); ES: entrance slit; CM1, 2: confocal mirrors; RG: reflective diffraction grating. The dashed line marks the lightproofed housing. (b) Setup change for transmission (C: sample cuvette), (c) reflection (FC: optical fibre coupling, F: optical fibre, RS: reflective sample), and (d) fluorescence measurements.

optical components, such as its inverse dependence on the width of the ES. The impact of doubling the focal length of CM1 and CM2 on the spectral resolution, as well as the role of light intensity on the CCD line array are well suited for a jigsaw classroom.

3. Assembly and components of the setup

Figure 2 shows a photograph of the major optical unit of the DIY C–T spectrometer. The mechanical structures of all components are built from commercial LEGO® bricks. The entire setup is mounted onto a LEGO® baseplate (alternatively, an optical breadboard [23] is used if the spectrometer has to be portable). Further components used are listed in table 1.

The confocal mirrors are purchased from a professional supplier of optical components, while the reflective diffraction grating is prepared from a commercial compact disc (CD). It features >85% reflectivity and groove distance accuracy (groove distance $d = 1.6\,\mu$m, 625 lines mm^{-1}) for the spectrometer. The ES is realized by two razor blades at adjustable distance (μm range). The CCD detector is based on a line scan camera module with a Toshiba sensor array (type 1304) and obeys a USB serial port for direct connection to a computer as well as a plug-and-play software for live view of the pixel values [24]. Note, that the Toshiba sensor is a standard in professional high-end spectrometers. The costs of the DIY C–T spectrograph accumulates to a maximum of about 500 Euros. Costs can be considerably reduced if students bring together most of the LEGO® bricks.

An end-to-end instruction with a detailed part lists of the LEGO® bricks is available open online, free of charge [25] (license: Creative Common 4.0 (CC BY-SA 4.0)) and was sketched using the open source software LDraw [26] and LPub3D [27] (Hardback edition: [28]).

4. Classroom experiences

4.1. *Atom emission spectroscopy*

A key application of the spectrometer is the application of the Bohr–Einstein frequency-relation for an optical transition in an atomic system

$$\Delta E = E_2 - E_1 = h\nu = E_{\text{Photon}} \tag{1}$$

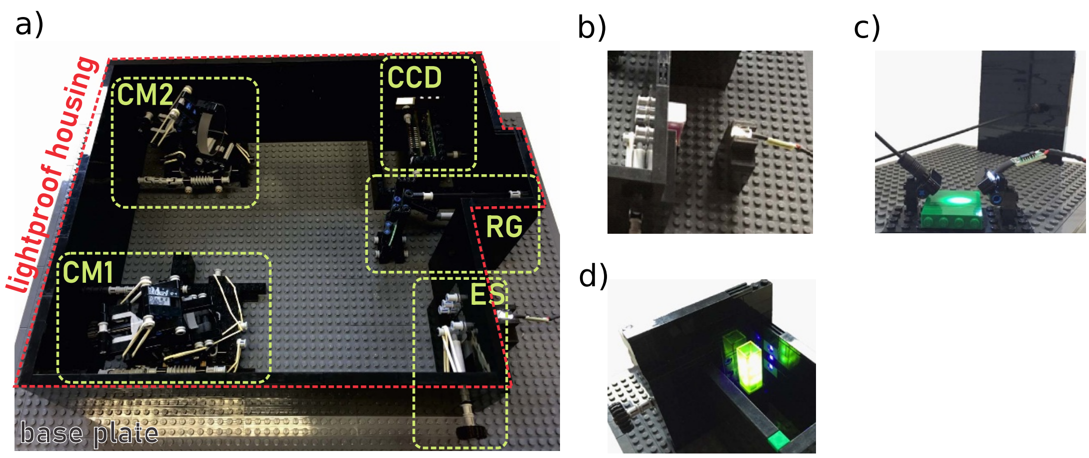

Figure 2. Photograph of the (a) major optical unit of the DIY Czerny–Turner spectrometer build from LEGO® bricks. The entrance slit is on the bottom right, the two confocal mirrors on the left and the CCD line array on the upper right (cf marks). (b) A close up of the entrance slit with adjustments for transmission measurements, (c) a close up of fibre coupling for reflection measurements and (d) a close up of the entrance slit with adjustments for fluorescence measurements.

Table 1. Optical and electronic components used in the spectrometer in reference to the online shops: www.amazon.de; www.thorlabs.de; www.eureca-messtechnik.de; www.conrad.de.

Component	Article	Distributor	Article number/ASIN
ES	Platinum razor blade	Amazon	B07KMKNHBR
CM1	1 Dielectric concave mirror 400–750 nm, $f = 200$ mm	Thorlabs Ltd	CM254-200-E02
CM2	2 Dielectric concave mirror 400–750 nm, $f = 200$ mm	Thorlabs Ltd	CM508-200-E02
RG	Intenso compact disc-RW 700 MB	Amazon	B000BV7AWE
CCD	Line scan camera module	EURECA Messtechnik GmbH	e9u-LSMD-TCD-1304-STD

using the spectrum of a 60 W mercury vapour light bulb (setup depicted in figure 1(b)). Here, E_{Photon} the photon energy of the incident light of frequency ν, h the Planck constant, and $E_{1,2}$ are two discrete energetic levels of the Hg atom with energy distance ΔE. For this purpose, the ES is narrowed to achieve the best possible spectral resolution. Figure 3 shows a typical line spectrum detected with the spectrometer and a CD as reflective diffraction grating.

A possible task for the students is to allocate the individual emission lines with atomic transitions of Hg as published in the literature and to calibrate the CCD line array, i.e. to assign a wavelength to each detector pixel. The inset of figure 3 depicts the magnified atomic Hg emission line at about 546 nm that is used to determine the full line width at the half value of the peak maximum (FWHM). The comparison with literature data (cf table 2) acts as starting point for a joint discussion of the students about measurement errors, error sources, and ways for optimizing the spectrometers precision. In a demand lesson (optional) a more precise calibration routine can be discussed based on a polynom function of third order. The data of figure 3 reveal a wavelength spacing ($\Delta\lambda$/pixel) of (0.06 ± 0.01) nm/pixel. Note that the inaccuracy of the peak position for the emission line at approx. 404 nm is by a factor of approx. 10 larger compared to the other peak position uncertainties. The reason for this is that only a small wavelength range (in this case centred

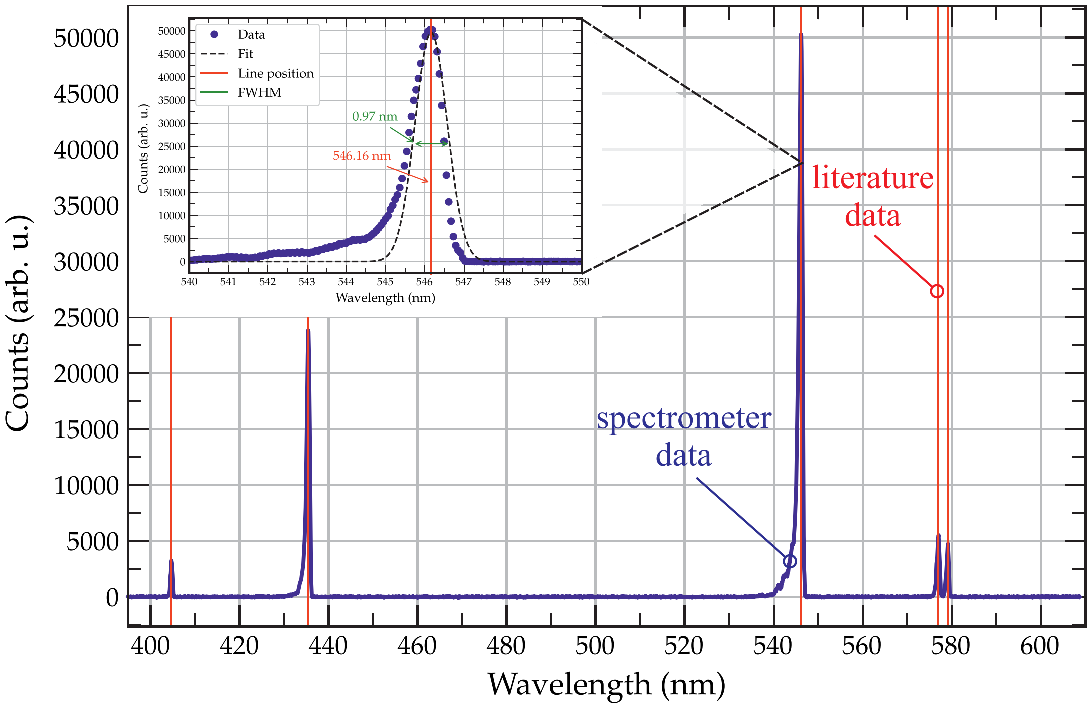

Figure 3. Atomic emission spectrum of a mercury vapour lamp as measured with the DIY Czerny–Turner spectrometer. Data points (blue), literature peak positions of atomic emissions (red). Inset: magnified peak of the emission line at 546.0735 nm (literature value, entrance slit approx. 80 μm). Gaussian fit to the data (black dotted line).

Table 2. Literature values of mercury emission line peak positions [29] in comparison to the determined peak positions and FWHM with their respective measurement errors.

Peak position: literature (nm)	Peak position: measured (nm)	FWHM (nm)
404.6563	(404.74 ± 0.12)	(0.56 ± 0.29)
435.8328	(435.41 ± 0.02)	(0.86 ± 0.05)
546.0735	(546.02 ± 0.01)	(0.98 ± 0.01)
576.9598	(576.93 ± 0.01)	(0.76 ± 0.21)
579.0663	(579.05 ± 0.01)	(0.61 ± 0.22)

at 580 nm) can be sharply imaged due to the grating properties in particular its curvature. As a consequence, the chromatic aberration increases with increasing distance to this wavelength. This aberration in combination with a small peak amplitude leads to a higher uncertainty in the fit and subsequently in the emission line peak position.

Note, that the DIY C–T spectrometer reveals a spectral resolution by a factor of at least 15 higher in comparison with previously reported self-made spectrometers (typically ranging from approx. 15–37 nm [6]). By utilizing a different grating, e.g. a blaze grating (article number GR25-1205, Thorlabs Inc.), it becomes possible to further increase the spectral resolution and especially the signal sensitivity.

4.2. Transmission, reflection and fluorescence spectroscopy

Figure 4 shows the measurement results obtained for determining (a) the transmission spectrum of potassium permanganate $KMnO_4$ (part (a) and (b)), (b) the fluorescence spectrum of fluorescein

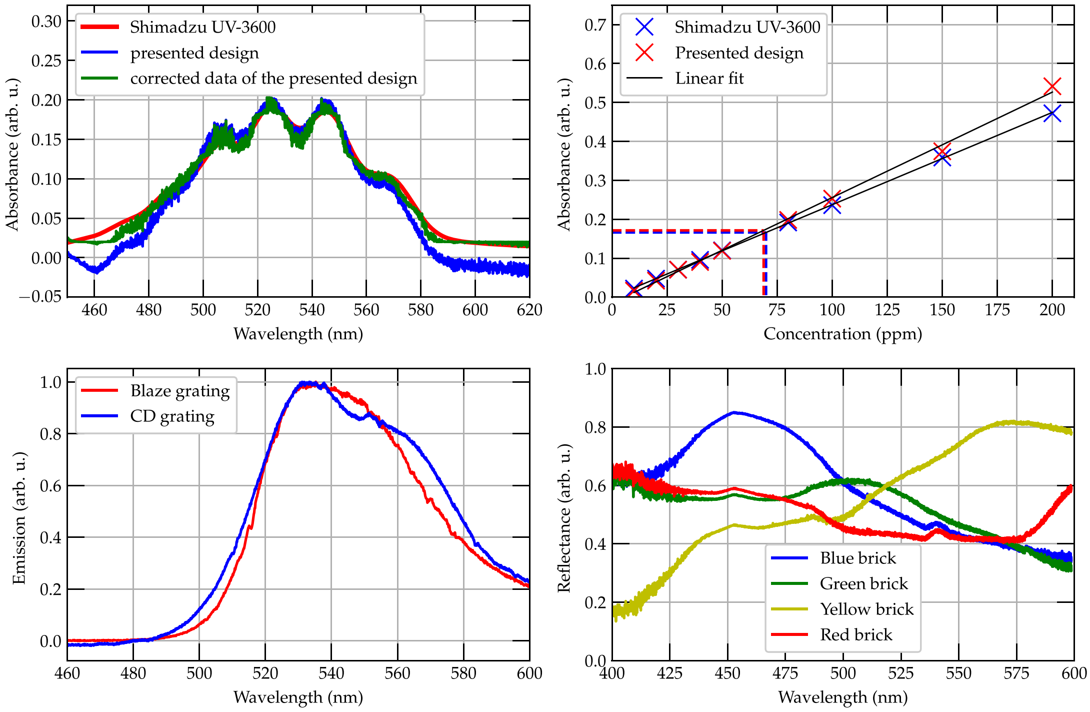

Figure 4. Classroom examples of the spectrometer. Top left: absorption spectra of potassium permanganate at a concentration of 80 ppm using the DIY Czerny–Turner spectrometer before (blue data points) and after (green data points) correction for the nonlinear signal response of the CCD sensor. For comparison, the spectrum measured with a high-end spectrometer (Shimadzu UV-3600, red data points) is plotted. Top right: absorbance as a function of concentration at 525 nm as being determined from the spectra of a series of potassium permanganate solutions. The calculated concentration of the unknown sample is marked with dotted lines. Bottom left: normalized emission spectra of fluorescein under exposure to UV light using a CD grating (blue) or blaze grating (red). Bottom right: reflection spectra of different coloured LEGO® bricks (blue, green, yellow and red).

and (c) the reflectance spectra of four differently coloured LEGO® bricks with the DIY C–T spectrometer—all of them possible in the framework of teaching lessons. For the individual measurements, the spectrometer setup was rebuild and experimentally prepared within less than 5 min in each case, i.e. it can be rebuild in the breaks between teaching lessons. All three measurements are directly related with applications as described in the following.

4.2.1. Transmission spectroscopy. The $KMnO_4$ transmission spectrum (figure 4 (top left)), shown for a concentration $c = 80$ ppm) is used in analytical chemistry courses to learn how an unknown concentration of a solution can be revealed. For this purpose, the students prepare a series of $KMnO_4$ solutions in purified water with concentrations in the range of 0, 10–200 ppm and fill it into a cuvette. A white light LED (cf. table 3) is used for illumination according to figure 2(b). They start to measure the transmitted intensity spectrum of purified water $I_0(\lambda)$ using the solution with $c = 0$ ppm. Then, the transmitted spectra $I_t(\lambda)$ are measured for each concentration and the spectral absorbance $\alpha(\lambda)$ is determined using Lambert–Beer's-law:

$$I_t(\lambda) = I_0(\lambda) \cdot \exp - (\alpha(\lambda) \cdot d). \qquad (2)$$

Here, d is the sample thickness along the direction of light propagation. Parallel to the analysis, the students may be motivated to discuss about the normalization procedure based on $I_0(\lambda)$ with the goal to understand that losses by cuvette and solvent are removed. Now, the absorbance is plotted as a function of concentration for a

Table 3. Components for transmission measurement in reference to the online shops: www.carlroth.com; www.conrad.com.

Component	Article	Distributor	Article number/ASIN
C	One use cuvette PMMA, Makro 2.5–4.5 ml	Carl Roth GmbH + Co. KG	Y196.1
LS	2 TRU COMPONENTS LED white $d = 5$ mm, 5000 mcd	Conrad Electronics SE	1573733

Table 4. Components for fluorescent measurement in reference to the online shops: www.carlroth.com; www.conrad.com.

Component	Article	Distributor	Article number/ASIN
C	One use cuvette PMMA, Makro 2.5–4.5 ml	Carl Roth GmbH + Co. KG	Y196.1
UV-LS	2 TRU COMPONENTS LED white $d = 5$ mm, 5000 mcd	Conrad Electronics SE	1573733

selected wavelength (preferred at one of the maxima of the spectra, e.g. 525 nm), as depicted in figure 4 (top right). A linear fit serves as calibration function for the determination of a $KMnO_4$ solution prepared by another group of students with unknown concentration.

Figure 4 (top left) also shows a spectrum of the DIY C–T spectrometer after correction for the nonlinear response of the CCD line array. For comparison, the spectrum of the same sample determined with a high-end spectrometer (type UV-3600 from Shimadzu) is plotted.

4.2.2. Fluorescence spectroscopy. Figure 4 (bottom left) shows the emission spectrum of a fluorescein solution (0.02% in purified water) that was determined using the principle setup depicted in figure 1(d). As for transmission measurements, the solution needs to be illuminated. In this case, however, an ultraviolet LS build of three 375 nm UV LEDs is used and the direction of exposure is orthogonal to the ES (cf. table 4).

An accompanying teaching lesson may address the difference between absorption and (spontaneous) emission according to Einstein's principle of light–matter interaction. As a result the students shall find-out the idea behind increasing the light power, choosing UV light and changing the direction of light propagation, i.e. excitation is required as additional step in emission spectroscopy. A topic for demand lessons is the conclusion of a lower photon energy of the emitted light in comparison with the excitation light that results in a major emission peak at about 535 nm.

Measuring fluorescence with a spectrometer also proofs to be more challenging than the measurement of a transmission spectrum from the experimental viewpoint. The reason is that the light emitted by the fluorescein solution is weak due to a low conversion efficiency ($\ll$1) of excitation and emission as well as due to diffusive emission. Figure 4 (bottom left) therefore shows the fluorescence spectrum of the fluorescein solution using two different reflective diffraction gratings: (a) the CD (blue data points) and (b) a blaze grating (red data point, blaze wavelength $\lambda_B = 500$ nm, 300 lines mm^{-1}, Thorlabs Inc. article number: GR25-0305). The latter reveals the fluorescein spectrum in full accordance with literature [30–32]. Note, that spectrum with the CD also reflects the majority of fluorescein emission features but shows a small dip at about 550 nm, that is a result of the absorption characteristics of the re-recordable CD itself. Students may study the relation of this dip to the grating by measuring the same spectrum subsequently with CDs from different distributors (also read-once, read-many, read-write media shall be compared).

Table 5. Components for reflection measurement in reference to the online shops: www.bricklink.com; www.amazon.com; www.conrad.com.

Component	Article	Distributor	Article number/ASIN
FC	Fibre optical coupler ('Spaltersatz')	Bricklink	See [25] for article numbers
F	iVANKY optical cable, Toslink cable, 1.8 m optical audio cable	Amazon	IVANKY-OC01
LS	2 TRU COMPONENTS LED white $d = 5$ mm, 5000 mcd	Conrad Electronics SE	1573733

4.2.3. Reflection spectroscopy. Figure 4 (bottom right) depicts the result of reflection spectra recorded for four LEGO® bricks of different colour. Here, the ES of the spectrometer is exchanged by a fibre optical (cf. table 5) coupler equipped with an optical fibre (figure 1(c)) to enable spectral detection at an angle according to the law of reflection. The white light LED is again used to illuminate the LEGO® bricks (45° angle of incidence).

A reference spectrum $P(\lambda)_{\text{reference}}$ is recorded using a white LEGO® brick, so that the reflectance $R(\lambda)$ can be calculated for the measured spectra $P_{\text{sample}}(\lambda)$ of each coloured brick using the relation [33]:

$$R(\lambda) = \frac{P(\lambda)_{\text{sample}}}{P(\lambda)_{\text{reference}}}. \qquad (3)$$

The results can be used in the classroom to discuss the possibility of automatic detection of plastic of different types in the context of waste separation, recycling, environment protection and micro plastics—one of the major applications of spectroscopy in these fields.

5. Conclusion and summary

We can conclude that it is possible to construct a DIY C–T spectrometer that matches the demands of classroom teaching in natural sciences and features a spectral resolution and sensitivity for atomic line emission spectroscopy using LEGO® bricks. The spectrometer thus represents another example of optics/photonics instruments/setups that can be realized with this approach and extends the series of educational setups from Michelson-interferometer [23], holographic recording setup [34], optical tweezer [25], laser powermeter [35] up to an intra-cavity, frequency-doubled Nd:YAG laser system [25]. From the technical viewpoint, the setup profits from the mechanical precision of the LEGO® bricks as a result of the superior competence of LEGO® systems A/S in the injection moulding technology. In the classroom, the use of LEGO® bricks is a major motivation factor for students, but the teaching lesson also profits from the distributed knowledge in mechanical building with LEGO®.

Another important feature for classroom applications is its quick and easy modularity, i.e. to the possibility to use the DIY C–T spectrometer for emission line, transmission, fluorescence and reflection spectroscopy. Thus, the setup is either well matched with the teachers' needs and boundary conditions of the day-to-day business, in particular taking short (minute-range) lesson preparation times into account. In addition, it turns out that the modularity also opens-up applications in rather different courses, disciplines and topics, ranging from physics, chemistry, biology, life sciences and related cross- and interdisciplinary topics. Here, the direct link with many state-of-the-art socio-economic applications shall be added besides the precision of fit with the curricula of modern natural sciences. But also the fact that one and the same system can be used by different teachers is not insignificant considering joined knowledge in handling and maintenance.

Finally, the low price of the DIY C–T design is striking for the application in many schools, thus, securing the hands-on experience of many students (world-wide) in spectroscopy.

To sum up, the presented DIY C–T spectrometer has the potential of becoming a workhorse in schools for the natural sciences. It combines modularity, high spectral resolution and sensitivity, supports students' motivation, matches with the teachers' needs, while remaining affordable to a large number of educational institutions.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Björn Bourdon studied physics at the University of Osnabrück from 2011-2016. Since his PhD in 2020 in the research group 'Ultrafast Physics' of Prof. Dr. Mirco Imlau, he completes his postdoc phase as project leader in the BMBF-funded project 'optocubes'.

Rasmus Böttcher studied mathematics and physics at the University of Osnabrück for the teaching profession at grammar schools. Following his studies, he completed his traineeship at the Studienseminar Braunschweig. He is currently a teacher of physics and mathematics at a high school in Braunschweig.

Mirco Imlau studied physics at the University of Cologne, wrote his doctoral thesis on the interaction of laser light with crystalline solid-state materials, and from 2002 specialized in the physics of (ultra-)short laser pulses within the framework of a junior professorship. He then held professorships at the University of Vienna and Université de Lorraine before being appointed Professor of Experimental Physics at the University of Osnabrück in 2008.

Marco Beeken studied chemistry and biology for the Gymnasiumlehramt in Oldenburg. After his doctorate in 2010 in the research group of Ilka Parchmann at the University of Oldenburg, he worked as a teacher in Rhauderfehn and Cloppenburg after his traineeship in Wildeshausen. Since 2018 he is professor for chemistry didactics at the University of Osnabrück.