Good Practice Report

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Studying the nomenclature of dioxins using a structure model kit based on electronic components linked with plastic tubes

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Abstract: Commercially available molecular models are elaborately made but generally expensive, which hinders their distribution to all classroom students. Aiming at developing an affordable molecular model, we developed a structure model kit consisting of inexpensive electronic components including transistors and colored light-emitting diodes (LEDs) with a total cost of *ca.* 2 USD. The structure model kit was designed for building a family of environmental pollutant molecules known as dioxins, in which transistor, white LED, red LED, and yellow LED components are used to represent sp^2 carbon, hydrogen, oxygen, and chlorine atoms, respectively. Herein, we report an activity directed to nonchemistry majors studying environmental science and electronic engineering to help them gain insight into the molecular structure of dioxins using the newly developed structure model kit. The activity was well received by many students, some of whom came to understand the relationship between the structure and nomenclature of dioxins, mainly 2,3,7,8-tetrachlorinated dibenzo-*p*-dioxin (2,3,7,8-TCDD) and its isomers.

Keywords: dioxins; isomer; molecular model; nomenclature.

1 Introduction

Owing to the high cost of commercially available molecular models, they are generally difficult to distribute to all classroom students. Therefore, some efforts have been devoted to the development of handmade molecular models that can be constructed from inexpensive materials (Chuang et al., 2012; Davis et al., 2010; Dragojlovic, 2015; Erlina et al., 2018; Horikoshi et al., 2021; Horikoshi et al., 2022; Marchak et al., 2021; Moreno et al., 2018; Siodłak, 2017; Turner, 2016). In this context, we were interested in designing a molecular model kit consisting of inexpensive electronic components including transistors, white light-emitting diodes (LEDs), red LEDs, and yellow LEDs, which are used to represent sp^2 carbons, hydrogens, oxygens, and chlorines, respectively, to visualize a family of environmental pollutants known as dioxins. Dioxins including polychlorinated dibenzo-*p*-dioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), and polychlorinated biphenyls (PCBs) are highly toxic compounds carrying chlorine atoms and benzene moieties, as shown in Figure 1 (Alaee, 2016; Schecter & Casiewicz, 2003).

PCDDs and PCDFs are generated as undesirable byproducts during many thermal and industrial processes. They are almost planar tricyclic aromatic compounds having a varying number of chlorine substituents between 1 and 8. Meanwhile, PCBs are used in numerous industrial applications owing to their insulating and

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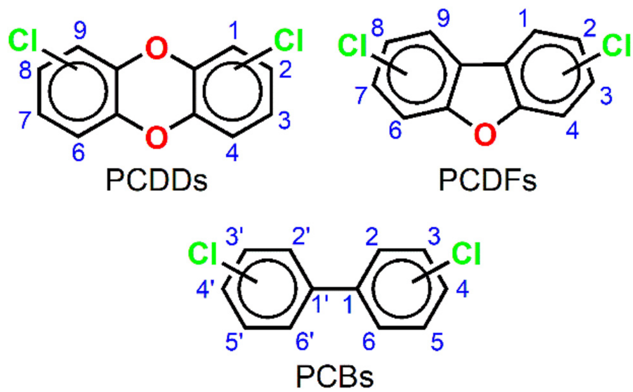

Figure 1: Schematic diagrams of polychlorinated dibenzo-*p*-dioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), and polychlorinated biphenyls (PCBs) with potential positions for substitution indicated by numbers. The number and positions of chlorine atoms are arbitrary.

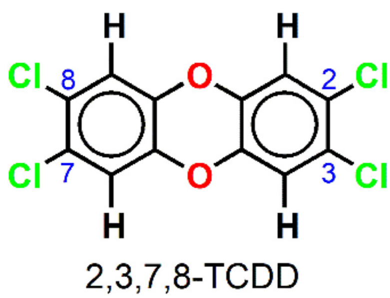

Figure 2: Schematic diagram of 2,3,7,8-tetrachlorinated dibenzo-*p*-dioxin (2,3,7,8-TCDD).

fire-retardant properties. Among the known dioxins, 2,3,7,8-tetrachlorinated dibenzo-*p*-dioxin (2,3,7,8-TCDD, Figure 2) is the most toxic and has been extensively investigated. 2,3,7,8-TCDD exhibits a highly symmetric structure and has harmful effects on humans, disturbing the normal function of human hormones and causing carcinogenicity and teratogenicity.

In this paper, we report an activity in which nonchemistry majors, i.e., environmental science and electronic engineering students, were requested to build dioxins, mainly 2,3,7,8-TCDD and its isomers, using the newly developed structure model kit based on electronic components. The structure model kit can also be used to model other environmental pollutants; however, considering the lecture time and the ability of the participants, we focused only on 2,3,7,8-TCDD and its isomers in this activity. The students had previously been taught about dioxins in an environmental science class; however, most of them did not know the molecular structures, isomerism, and nomenclature of dioxins. This activity provided the students with an opportunity to learn the relationship between the isomeric structures and nomenclature of simple aromatic compounds and dioxins. This activity was conducted as a remote lecture in 2021 during the COVID-19 pandemic and as a face-to-face lecture in 2022 once the COVID-19 pandemic was under control. Because the molecular model kit based on electronic components was lightweight, it could be mailed to students in advance for the 2021 lecture.

2 Materials

Figure 3 shows the materials used to construct the structure model kit, which were 12 transistors, 9 white LEDs, 2 red LEDs, 6 yellow LEDs, 12 black heat-shrink tubes, 12 silicone tubes, and 2 rubber gaskets. The white LEDs in this text refer to the red LEDs with the colorless capsules. The latter is less expensive than the former. Prior to their distribution to the students, the electrodes of all the electronic components were cut and spread, and the plastic tubes were cut to a width of 13 mm. The correspondence between electronic components and chemical elements is also shown in Figure 3. The rubber gaskets represent the resonance hybrid structure of benzene. The total cost of each structure model kit was *ca.* 2 USD. Figure 3(c) shows how to connect the electronic components.

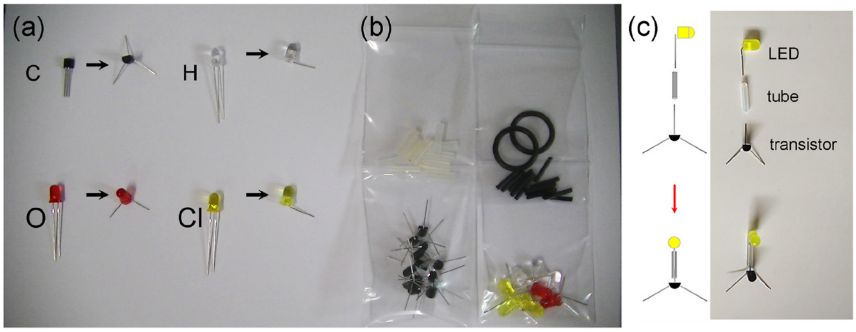

Figure 3: Materials of structure model kit (a) Electronic components before and after processing, (b) structure model kit distributed to students, and (c) method of connecting electronic components.

3 Activity overview

This activity was designed to cover two 90 min lectures and to provide nonchemistry majors with an opportunity to learn the nomenclature of simple aromatic compounds and dioxins, mainly TCDD analogues, by building their own structure models. Before conducting this activity, the students were made familiar with isomers and skeleton diagrams of benzene derivatives. PowerPoint slides providing a brief description and detailed instructions for building the dioxin models, together with the handout given to each student, are included in the Supplementary Information.

The definition of isomerism and the corresponding nomenclature rules were briefly explained using pre-constructed chlorobenzene and 1,2-dichlorobenzene models (Figure 4a and b), after which the students were asked to build 1,3- and 1,4-dichlorobenzene models (Figure 4c and d). Next, dioxins, mainly their structural features and nomenclature rules, were introduced to the students using PowerPoint slides and the corresponding structure models. Subsequently, the students were required to build the structure models for 2,3,7,8-TCDD and 1,2,4,9-TCDD (Figure 5). It was explained that 2,3,7,8-TCDD is extremely toxic to certain kinds of laboratory animals (Emsley, 1996). In both the remote and face-to-face lectures, the students took photographs of their TCDD models and attached them to reports they would later submit. In the final part of the activity, students were asked to name two TCDD isomers (1,3,6,9- and 1,3,7,8-TCDD isomers) depicted in the worksheet.

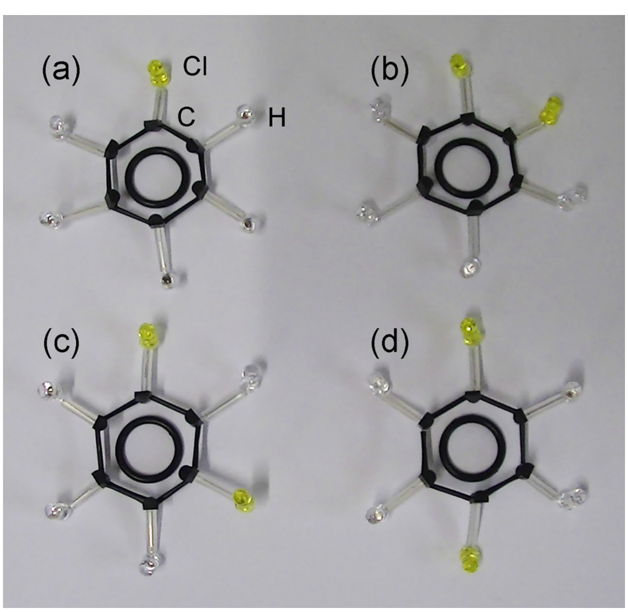

Figure 4: Structure models of (a) chlorobenzene, (b) 1,2-dichlorobenzene, (c) 1,3-dichlorobenzene, and (d) 1,4-dichlorobenzene.

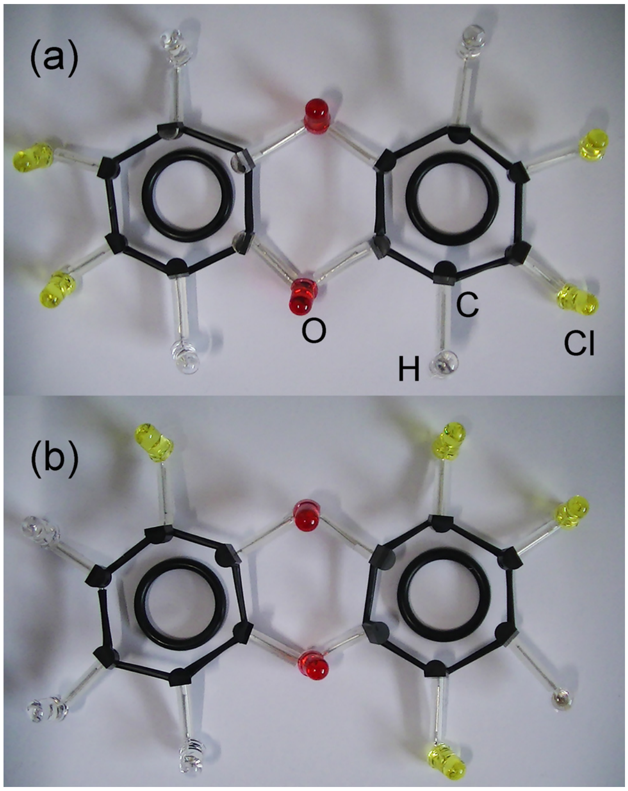

Figure 5: Structure models of (a) 2,3,7,8-tetrachlorinated dibenzo-*p*-dioxin and (b) 1,2,4,9-tetrachlorinated dibenzo-*p*-dioxin.

4 Results and discussion

The structure model kit cannot represent the exact bond lengths or angles of organic compounds because of their simple structure; however, these components are suitable to represent the isomers of simple organic compounds such as dioxins because the constituent elements can be easily detached and attached. This constitutes an advantage over commercially available ball-and-stick models, which occasionally break when the bond is removed. However, although the length of the LED electrodes may be varied to represent the actual size of the hydrogen, oxygen, and chlorine atoms, the differences between these atoms are not noticeable in this model. Because the transistors representing carbon atoms have only three electrodes, the structure model kit can only represent planar molecules containing sp^2 carbons and, therefore, it cannot be used to construct dichlorodiphenyltrichloroethane (DDT) and other pollutants containing sp^3 carbons. The use of heat-shrink tubes to construct the benzene rings in the structure model kit is not strictly necessarily. Instead, silicone tubes could be used without using a hair dryer or a toaster oven, which is required in the case of the heat-shrink tubes. However, the structure became somewhat fragile when substituents were removed from the benzene rings linked with silicone tubes; hence, heat-shrink tubes are recommended to connect the transistors.

This activity was aimed at nonchemistry majors comprising environmental science and electronic engineering students in their second semester. While the environmental science students learned about landscaping and environmental planning after promotion, the electronic engineering students focused on electronic materials and communication engineering. However, in their first semester, they mostly studied basic subjects, leading them to be unfamiliar with environmental science. In addition, although most environmental science majors studied chemistry during high school, most electronic engineering majors did not do so. Nevertheless, many of these students studied basic chemistry in their first semester, where they learned about isomerism and the skeletal structures of simple aromatic compounds. Moreover, they had learned in their first semester

Table 1: Percentage of correct answers for exercises submitted by the students (exercise numbers correspond to those on the worksheet).

Exercise	Environmental science majors		Electronic engineering majors		Total	
	2021 (*N* = 28)	2022 (*N* = 17)	2021 (*N* = 62)	2022 (*N* = 86)	2021 (*N* = 90)	2022 (*N* = 103)
1	100 %	100 %	100 %	100 %	100 %	100 %
2	100 %	100 %	100 %	97 %	100 %	96 %
3(a)	–	71 %	–	6 %	–	16 %
3(b)	–	100 %	–	89 %	–	91 %

that dioxin is an environmental pollutant. However, they were still not aware of its structure, much less its isomer.

The activity was held as a remote lecture in 2021 and a face-to-face lecture in 2022 (Table 1). The 2021 lecture participants comprised 28 environmental science majors and 62 electronic engineering majors. Meanwhile, 17 environmental science majors and 86 electronic engineering majors participated in the 2022 lecture. In the remote activity conducted in 2021, many students correctly constructed directed isomer models (Exercise 2 in the Supplementary Information). That is, the students had a high rate of correct answers when they were tasked with deriving the structure from the name of a TCDD isomer. Therefore, during the face-to-face activity performed in 2022, we created a slightly more challenging exercise (Exercise 3 in the Supplementary Information) in which the students were asked to name the isomers from their structural formulas. Disappointingly, the accuracy rate was as low as 16 % (Table 1) as most students answered 1,4,6,8- or 2,4,6,9-TCDD instead of 1,3,6,9-TCDD because they found the rule of using the lowest numbers to indicate a position difficult to understand. In the case of 1,2,7,8-TCDD, however, a literature review revealed that 1,2,7,8-TCDD and 2,3,6,7-TCDD could be used (Panteleyev & Bickers, 2006). Therefore, the 72 students who answered 2,3,6,7-TCDD were also correct. Overall, the higher accuracy rate of the environmental science majors could be attributed to the fact that they were generally more concerned about environmental issues than the electronic engineering majors.

From these investigations, we also speculate that the lower rate of correct answers in Exercise 3 was due to the following reasons: When we explained the numbering of dichlorobenzenes as an example at the beginning of the lecture, we numbered it clockwise from the top; this approach was probably in the minds of some of the students, which could explain why some students numbered it from the upper-right or upper-left carbon without flipping the molecule. This mistake was within our expectations and we thoroughly explained it to the students. However, the exercise of flipping molecules up, down, left, right, and then numbering proved difficult for nonchemistry majors to grasp.

The development of molecular models composed of inexpensive materials including origami paper craft (Davis et al., 2010), foamed polystyrene balls (Erlina et al., 2018), clay (Marchak et al., 2021), beads (Chuang et al., 2012), pipe cleaners (Turner, 2016), straws (Moreno et al., 2018), whiteboard markers (Dragojlovic, 2015), and bottle caps (Siodłak, 2017) has been extensively reported. These materials provide an excellent and simple means to construct molecular models that can be easily assembled by students. Similarly, our models based on electronic components are easy to assemble. Nonetheless, the combination of commercially available molecular models and computer software would be helpful to teach exact molecular structures. More recently, outstanding lectures on three-dimensional printed molecular models (Penny et al., 2017) and models displayed on smartphones (Eriksen et al., 2020) have been provided; however, the production and distribution of such teaching aids is difficult. Conversely, handmade molecular models are simple and accessible tools that are readily available for use.

Planar molecules such as dioxins can be constructed with clay and toothpicks, which are less expensive than our models based on electronic components. However, clay is uncomfortable to handle; students might not like using clay with their hands because their computers and smartphones get dirty. Moreover, clay is difficult to color, and representing different elements (carbon, hydrogen, oxygen, and chlorine) using uncolored clay is challenging. In contrast, electronic components can be conveniently handled, and LEDs are commercially available in white, red, yellow, blue, and green colors. Therefore, the molecular model kit based on electronic components is suitable for this activity. It should be noted that in this structure model, the resonance hybrid structure of the benzene ring is represented by a rubber gasket, and the instructor should emphasize that students should not mistake the gasket for the π orbital of the benzene ring.

5 Hazards

All electronic components used in this study are RoHS-compliant and do not contain dangerous substances. However, some of the electronic components contain sharp electrodes that should be handled with care. Instructors should take care when cutting the electrodes with snips and the plastic tubes with scissors. Hair dryers and toaster ovens should be also handled with caution because they can cause burns. Moreover, a microwave oven should not be used when securing the transistor with a heat-shrinkable tube because the transistor may burst.

6 Conclusions

We have developed a structural model kit consisting of inexpensive electronic components, which is easy to use in remote lectures. Activities using this structure model kit provide nonchemistry majors with an excellent opportunity to learn the isomerism and nomenclature of aromatic compounds. Some of the students that attended the activity were able to understand the relationship between the structure and nomenclature of simple organic compounds and some dioxins.

Supplementary information

The following supplementary information is also provided: PowerPoint slides, detailed instructions, and student handout.

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Supplementary Material: This article contains supplementary material (https://doi.org/10.1515/cti-2022-0051).