Good Practice Report

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Learning with NanoKid: line-angle formula, chemical formula, molecular weight, and elemental analysis

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Abstract: The conversion from line-angle formula to chemical formula often poses a challenge for first-year nonchemistry majors. To address this, the authors developed an engaging exercise lecture that encompasses the conversion process and related chemistry concepts, including molecular weight and elemental analysis. Initially, the instructor reviews basic chemistry concepts with the students. Subsequently, students construct a NanoKid structure model using transistors and red LEDs connected by plastic tubes, representing carbon and oxygen atoms, respectively. By referencing their models, students identify the chemical formula of NanoKid, calculate its molecular weight, and perform elemental analysis under the guidance of the instructor. Additionally, they estimate the scale of the NanoKid model relative to the actual NanoKid molecule. The exercise promotes peer review among students and is completed within approximately 45 min. A post-lecture questionnaire revealed that the exercise was well-received by the students.

Keywords: line-angle formula; chemical formula; molecular weight; elemental analysis

1 Introduction

Line-angle formulas (skeletal formulas) are commonly used in general chemistry textbooks to depict complex organic compounds, aromatic compounds, and carbohydrates. However, first-year nonchemistry majors often struggle with these formulas, finding it challenging to interpret them and to convert them into chemical formula (Figure 1). Recognizing the importance of understanding line-angle formulas and calculating molecular weights for chemistry education, the authors devised an engaging exercise lecture centered around NanoKid (Figure 2). Students participating in the exercise lecture will subsequently engage in the synthesis of acetylsalicylic acid, including yield calculations. However, accurate yield determination will be compromised if they are unable to convert line-angle formulas into chemical formulas and subsequently to molecular weights. In standard textbooks, the benzene motifs of salicylic acid and acetylsalicylic acid are typically represented using line-angle formulas. NanoKid, a molecule synthesized by Professor Tour and colleagues, features a human-like structure in its line-angle formula representation and includes various types of carbon such as acetylene (sp carbon), benzene ring (sp^2 carbon), and methyl group (sp^3 carbon) (Chanteau & Tour, 2003; Chanteau et al., 2003). This diversity makes NanoKid an ideal subject for elucidating the conversion process. Given the high cost and distribution

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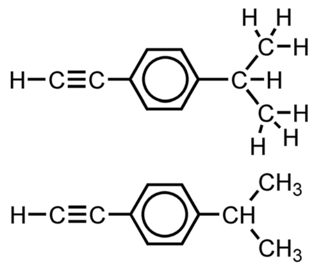

Figure 1: Depiction of 1-ethynyl-4-*i*-propyl-benzene in (a) structural, (b) condensed, and (c) line-angle formulas.

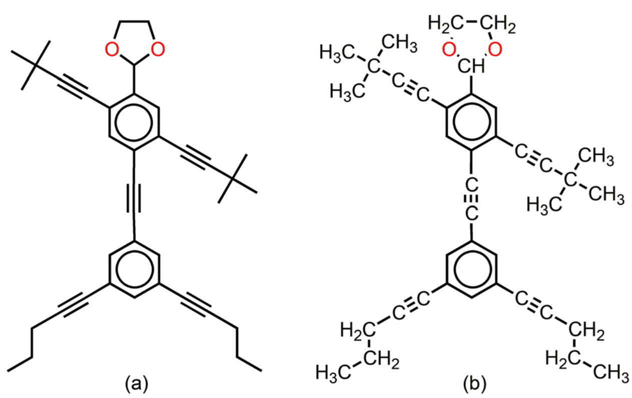

Figure 2: Representation of NanoKid in (a) line-angle and (b) condensed formulas.

challenges of commercial molecular models, the authors designed an affordable NanoKid molecular model using basic electronic components. This paper presents the structure of the exercise lecture designed for first-year nonchemistry majors, which comprises a brief review of chemical bonds, construction of the NanoKid molecular model, identification and counting of NanoKid's chemical formula, calculation of its molecular weight and elemental analysis, and a comparison of the model's size to the actual molecule. Feedback from a questionnaire administered immediately after the lecture indicates that the exercise was engaging and informative for the students.

2 Lecture overview

The exercise lecture was designed to last approximately 90 min. Detailed information on the teaching materials provided to the students and the construction of the NanoKid model can be found in the Supporting Material. The participants were first-year nonchemistry majors, specifically from environmental science and electronic engineering disciplines, totaling 75 students divided into 5 groups. Many of these students were not proficient in chemistry, often due to not having chosen it as a subject for their college entrance examinations.

The lecture commenced with a review of fundamental concepts, including the valence electrons of carbon, hydrogen, and oxygen, which are 4, 1, and 2 respectively, allowing these elements to form the corresponding number of covalent bonds per atom (Figure 3a). It was highlighted that in line-angle formulas, the representations of carbon and hydrogen are omitted, with carbon atoms implied at line segments, corners, and intersections (Figure 3b). Additionally, the C–C bonds in a benzene ring are not alternating single and double bonds but are instead characterized by 1.5 bonds, forming a regular hexagon (Figure 3c).

Before distributing the materials for the molecular model (Figure 4a), the instructor outlined the assembly rules. The principle was straightforward: connect all electrodes of the provided parts, ensuring they are encased

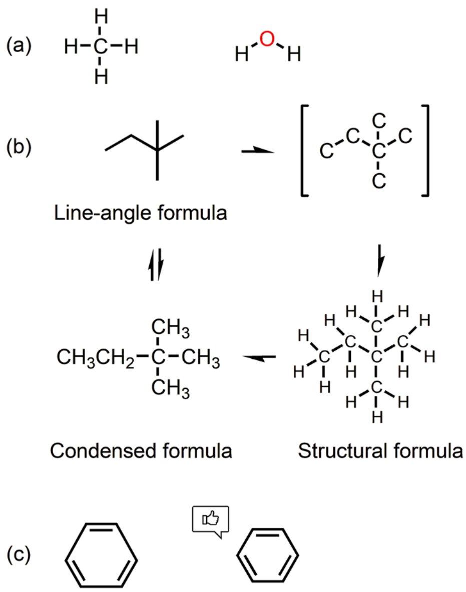

Figure 3: Overview of chemical bonds: (a) bond orders, (b) depiction in line-angle formula, and (c) the 1.5 bond characteristic of benzene.

within plastic tubing (Figure 4b). In the model, transistors and red LEDs symbolize carbon and oxygen atoms, respectively, while colorless, black, and red plastic tubes represent single, 1.5, and triple bonds, respectively. Each student constructed their own molecular model, resulting in various isomers of NanoKid (Figure 4c), with some accurately replicating the NanoKid structure. Students who initially built isomer models were encouraged to adjust their creations to match the NanoKid molecular model (Figure 4d). Only a few students were familiar with NanoKid prior to the lecture.

Following the construction of the models, students were tasked with identifying the composition of NanoKid by examining their models, specifically the types of atoms present and their quantities. This process was repeated until accurate compositions were achieved, with peer review among students facilitating correct responses. Details of the peer review are provided in Supporting Information. Subsequently, they calculated the molecular weight and performed elemental analysis for NanoKid. Finally, the students estimated the scale of their molecular model relative to the actual NanoKid molecule, enhancing their understanding of molecular dimensions. As students engage in the exercise, instructors should clarify that, according to molecular modeling calculations, the five-membered ring containing two oxygen atoms, which represents the head of NanoKid, is not flat (as referenced in the NanoPutians Wikipedia article). Therefore, it is practically challenging to directly compare the dimensions of the NanoKid model with the actual NanoKid molecule.

3 Results and discussion

The exercise lecture incorporated student peer review, enhancing the learning experience for both the reviewers and those being reviewed. This approach significantly contributed to the majority of students correctly completing the exercises. As anticipated, interpreting line-angle formulas to count chemical formulas proved challenging for the students. A common error involved miscounting the number of hydrogens attached to carbon atoms in the benzene ring, with some students assuming two hydrogens per carbon. This misconception might have stemmed from the electronic component-based NanoKid model, where the benzene ring is depicted by a rubber ring within a hexagon formed by six transistors, as illustrated in Figures 2 and 4d. The students' unfamiliarity with the conventional representation of benzene – a hexagon with a circle – likely led to these errors. Interestingly, only a few students neglected to count the hydrogen atoms attached to the sp^3 carbon in NanoKid's chin.

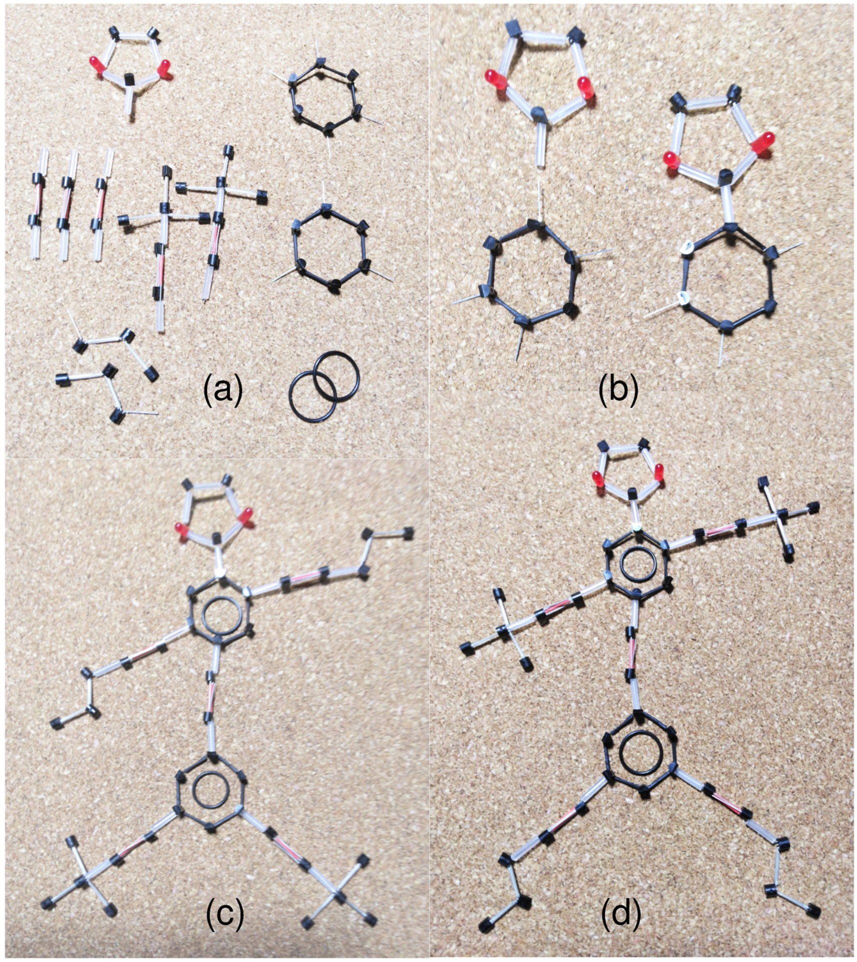

Figure 4: Construction of the NanoKid molecular model using electronic components: (a) assembly materials, (b) method of joining parts, (c) an example of incorrect isomer models, and (d) the accurate NanoKid model. Transistors represent carbon atoms, red LEDs represent oxygen atoms, and transparent, black, and red plastic tubes denote single, 1.5, and triple bonds, respectively.

While many students initially struggled with counting chemical formula, they swiftly and accurately completed the calculations for molecular weight and elemental analysis, thanks to the peer review process and guidance from the instructor. However, few students could accurately determine the scale of the molecular model relative to an actual molecule. The primary difficulty lay in comparing magnitudes, specifically between 10^{-2} m (cm) and 10^{-9} m (nm), a task made challenging by their reliance on digital calculators and infrequent practice with manual calculations.

To assess their understanding further, the instructors tasked the students with identifying the composition and calculating the molecular weight and elemental analysis of NanoJester (Chanteau & Tour, 2003; Chanteau et al., 2003), a molecule related to NanoKid, presented in line-angle form. An impressive 96 % of the students completed this task successfully.

While it is possible to use more common molecules than NanoKid to teach structural formulas, molecular weights, and elemental analyses, the construction of the NanoKid model was deliberately chosen for this exercise. The aim was to make chemistry engaging by involving students in building molecular models. The post-lecture questionnaire results indicated that this approach was well-received, suggesting that the inclusion of student peer review might have also positively influenced the students' enjoyment of the lecture.

Molecular models are highly effective tools for understanding the structure and composition of molecules. However, commercially available models are often prohibitively expensive and impractical for use by every student in a classroom setting. To address this issue, the authors previously developed molecular models using inexpensive electronic components to represent atoms (Horikoshi et al., 2022; Horikoshi et al., 2023a; Horikoshi et al., 2023b). In this system, transistors represent carbon atoms, and LEDs of different colors correspond to

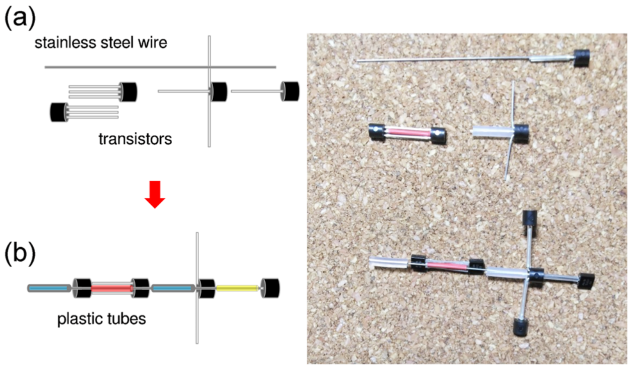

Figure 5: Representation of sp^3 carbon using transistors, stainless steel wire, and plastic tubes: (a) before and (b) after assemble.

various heteroatoms. These components are linked by plastic tubes to create a molecular model. For instance, the NanoKid model, which consists of 39 carbon atoms, can be assembled using these electronic components at a cost of approximately 1.0 USD, with a compact total length of approximately 20 cm.

While these electronic component-based molecular models do not accurately represent bond lengths and angles and are somewhat fragile, their low cost and small size make them suitable for illustrating the line-angle structures and compositions of large molecules. Their ease of repair allows for repeated use. The transistor's three electrodes can be adapted with the addition of a stainless wire (Figure 5) to represent the tert-butyl group $(CH_3)_3C$–, akin to the NanoKid's hand. However, the molecular model struggles with molecules like styrene, where a benzene ring (bond order of 1.5) and an alkene (bond order of 2) coexist, primarily because it becomes challenging for students to differentiate these components using the molecular model.

Developing affordable molecular models that can be distributed to all students is a significant challenge in chemistry education. Various inexpensive materials, such as beads (Chuang et al., 2012), foam balls (Dang et al., 2024), ping-pong balls (Elsworth et al., 2017; Horikoshi et al., 2021a; Horikoshi et al., 2021b), plastic drinking straws (Moreno et al., 2018), plastic bottle caps (Siodłak, 2017; Zhuo & Liang, 2023), neodymium magnets (Kao et al., 2015), and interlocking building blocks (Horikoshi, 2021), have been utilized to create molecular models. However, constructing large molecules with these materials results in unwieldy models. In contrast, large molecular models made from electronic components remain relatively compact.

4 Hazards

When handling the sharp wires and electronic component electrodes, caution is necessary to prevent injury. A hair dryer or toaster oven should be used to shrink the heat-shrink tubes. Caution should be exercised to avoid burns while handling electronic components and tubes post-heating.

5 Conclusions

Converting line-angle formulas to chemical formulas poses a challenge for many nonchemistry majors. To address this, the authors designed an engaging exercise lecture centered around building the NanoKid structure model using electronic components. The tangible aspect of the NanoKid model effectively engaged students, making the learning process enjoyable, particularly for digital natives who may have limited experience with hands-on activities. The incorporation of student peer review fostered communication among students and contributed to a dynamic learning environment. The authors are committed to further developing exercise lectures that utilize cost-effective molecular models accessible to all classroom participants.

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