

ACE, an online organic chemistry exercise platform with intelligent review function.  
Introduction to organics and its application in teaching

### Abstract

In organic chemistry exercises and test questions, students are usually required to draw the structure of the reaction product, the reaction mechanism and the synthesis route, etc. There is no platform in China that can answer the above questions online and make correct judgments on the answers.

ACE Organic (Achieving Chemistry Excellence: Organic Chemistry) is an online organic chemistry exercise platform with intelligent feedback function. After students use the drawing software in the system to complete the homework assigned by the teacher online, the platform will judge whether the student's answer is correct and give evaluation and prompts to guide students to solve the problem correctly. For complex mechanism and synthesis questions, ACE can accept multiple correct answers. By checking the statistics of the system, teachers can understand the students' mastery of knowledge points at any time. ACE has a forum to facilitate interaction between teachers and students. Teaching practice has proved that the openness of ACE has effectively improved students' interest in learning organic chemistry and cultivated students' rigorous scientific attitude.

The teaching content of organic chemistry is complex. After-class exercises not only help students deepen their understanding of the knowledge points they have learned, but also help students sort out their ideas and flexibly apply the knowledge they have learned to solve complex problems. Therefore, after-class exercises and tests are an important part of the basic organic chemistry course. With the development of network technology and the development of online teaching, online exercises have received more and more attention. Compared with the traditional written exercise mode, organic chemistry online exercises have many advantages: [1–4] Using drawing software to answer questions, students are required to answer more standardized questions; after answering questions, students can get immediate feedback and guidance; submitting homework is no longer restricted by time and place; through the statistical data provided by the system, teachers can understand students' learning situation more timely and accurately; teachers can use the time saved from correcting homework to interact with students and improve teaching effectiveness.

In recent years, some online learning programs for organic chemistry based on the Internet have been developed at home and abroad[5-10] to help students learn organic chemistry independently, and have achieved good teaching results. ACE: Organic Chemistry (Achieving Chemistry Excellence: Organic Chemistry, ACE [9]) is an organic online exercise platform jointly developed by Professor Robert B. Grossman of the Department of Chemistry and Professor Raphael Finkel of the Department of Computer Science at the University of Kentucky and published by Pearson Education, published as an organic online exercise platform. Compared with other online organic chemistry exercises, ACE has the advantage that ACE is one of the most intelligent online organic chemistry exercise

systems. Using the commonly used free software Marvin JS for drawing, teachers and students can use it online without installing the software on their computers. ACE's intelligent feedback system can not only determine whether the student's answer is correct, but more importantly, after the student's correct answer, ACE will prompt the key points of knowledge involved in the question, and after the wrong answer, ACE will point out the reason for the error. ACE is the only platform that can provide multi-step solutions to reaction mechanism and synthesis questions. It can intelligently distinguish multiple possible reaction mechanisms and multiple reasonable synthesis routes, and accept multiple reasonable answers. Teachers can clearly understand students' homework completion and knowledge mastery through ACE's automatic grading function without having to review homework one by one. ACE has built a communication platform for teachers and students. Students can ask questions in the forum and get replies from teachers or other students. In addition, ACE has a massive question bank with more than 2,600 exercises covering a variety of question types including reaction questions, naming questions, mechanism questions, synthesis questions, and multiple-choice questions. ACE has been translated into Portuguese and Chinese. It is one of the most widely used online organic chemistry study question systems and the only foreign online organic chemistry study question system with a Chinese version.

## 1. Introduction to use

### 1.1 Student interface

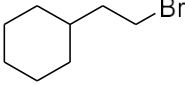
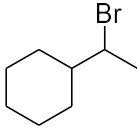
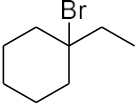
First, students can learn how to use the Marvin JS software and how to solve different types of exercises through the course guide (Tutorial course) [12]. While completing the exercises, students can also learn how to use the software to draw organic molecular structures in advance, which will prepare them for future scientific research and work.

The screenshot displays the ACE Organic student interface. At the top, there is a green header with the ACE Organic logo and navigation buttons: "我的课程" (My Course), "个人资料" (Personal Information), and "退出" (Logout). Below the header, a sub-header indicates the course level: "有机化学-19级" (Organic Chemistry-19th Grade). A secondary navigation bar contains buttons for "课程主页" (Course Home), "任务" (Tasks), "成绩册" (Gradebook), "教材" (Textbook), and "论坛" (Forum).

The main content area is divided into two panels. The left panel, titled "烯烃" (Alkenes), contains the text "每个问题的最大允许尝试次数: unlimited" (Maximum allowed attempts per question: unlimited) and a question: "(2) 下列反应的主产物是什么?" (What is the main product of the following reaction?). Below the question is a chemical reaction diagram showing cyclohexylmethene reacting with HBr. A link "Launch MarvinJS™ viewer or click image to copy source" is provided. The right panel is the Marvin JS drawing tool, which includes a toolbar on the left, a central canvas with the Marvin JS logo, and a vertical element palette on the right. At the bottom of the interface, there is a prompt "请提交您的第一个回答。" (Please submit your first answer.) and buttons for "试题列表" (Question List), "任务目录" (Task Directory), and "提交回答" (Submit Answer).

Fig. 1 Student answering interface in ACE

Table 1. ACE responses to different responses to the reaction of cyclohexylethylene with hydrogen bromide.

| answer                                                                            | ACE feedback                                                                                                                                                                                                                    |
|-----------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|  | There is no free radical initiator present, so the reaction is presumed to undergo an ionic mechanism, keeping in mind Markovnikov's rule.                                                                                      |
|  | A good answer, but not quite correct. You get the intermediate that gives you the compound, but the carbocation rearranges to give a more stable carbocation, so the Br atom in the product is not attached to the right place. |
|  | Correct, the initially formed secondary carbocation undergoes a 1,2-hydrogen shift (rearrangement) to give a tertiary carbocation.                                                                                              |

After the teacher assigns homework, students need to complete all exercises within the specified time and number of attempts. Students use MarvinJS to draw the molecular structure of the product and submit their answers (Fig. 1). The system will immediately give comments: if the answer is correct, the system will prompt the correct solution to the question to prevent students from "guessing"; if the answer is wrong, the system will point out the reason for the error based on the student's answer and guide the student to find the correct solution. Table 1 lists a reaction question: "Write the reaction product of cyclohexylethylene and hydrogen bromide (Fig. 1)." ACE provides feedback on three possible answers. For complex mechanism questions and multi-step synthesis questions, ACE can provide up to 20 pieces of feedback, which can basically review all the answers that students may submit. Therefore, ACE can help students to "know the reason and the reason" when answering questions. In particular, for more complex mechanism and synthesis questions, ACE will highlight its smartness. ACE can even "find" the mistakes in a certain step of the student's answer. For example, ACE will tell the student the wrong intermediate structure, charge, carbon skeleton or stereostructure, etc. With this targeted prompt, students can deepen their correct understanding of the knowledge points.

Outside of the designated time and number of attempts, students can still review previously completed questions through the "Practice Mode". This is the same as the assignment answering method, except that it is not included in the grade, making it convenient for students to use when reviewing.

## 1.2 Teacher interface

Teachers can choose questions from the question bank to assign homework to students (Fig. 2). The question bank of ACE is classified according to chapters. There are 35 chapters in total, such as acids and bases, alkanes, alkenes, alkynes, benzene and

derivatives, carbonyl compounds, etc. Each chapter is divided into different sections according to knowledge points and question types. For example, the chapter on alkenes is divided into different sections such as nomenclature, electrophilic addition, olefin oxidation, olefin retrosynthesis, mechanism and multi-step synthesis. The questions in the question bank come from the after-class exercises in various versions of Bruice[13] and Wade[14] and Grossman's "The Art of Writing Organic Reaction Mechanisms"[15], as well as the exercises written by the teachers who developed ACE. There are currently more than 2,600 exercises. When teachers select questions for students, they can set parameters such as the deadline for completing the questions, the maximum number of attempts allowed for each question, whether it is a timed test, and the scoring rules (Fig. 3).

The screenshot displays the ACE Organic Teacher Topic Selection Interface. The interface is organized into several functional areas:

- Top Navigation Bar:** Includes the ACE Organic logo and buttons for '我的课程' (My Course), '个人中心' (Personal Center), '试题库' (Question Bank), '教材' (Textbook), '交叉课程报告' (Cross-course Report), and '导出' (Export).
- Left Panel (题库试题):** Contains a dropdown menu for '选择主题' (Select Topic) and '选择问题设置' (Select Question Settings). Below this, it lists 'Alkenes, Electrophilic additions' with a note about the problem set (Prob 1-9: Bruice4 chap 4.33abcd, 35cgin).
- Central Panel:** Displays a list of questions for selection. Each question entry includes a checkbox, a question ID (e.g., #684, #685, #686, #687), and a brief description. The chemical structures of the reactants are shown, along with the reagent HBr.
- Right Panel (当前任务):** Shows the details of the current task, including the title '命名作业' (Naming Assignment), a description box, and a table for selecting questions. The table has columns for '选择' (Select), '分数' (Score), and '分' (Points).
- Bottom Bar:** Contains buttons for '全部' (All), '增加选项' (Add Option), '删除选项' (Delete Option), '关闭' (Close), '保存' (Save), and '保存并继续' (Save and Continue).

Fig. 2. Teacher topic selection interface in ACE

## 编辑任务

|                                             |                                         |                                                                                      |
|---------------------------------------------|-----------------------------------------|--------------------------------------------------------------------------------------|
| 姓名:                                         | 期末综合练习                                  |                                                                                      |
| 对学生可见?                                      | <input checked="" type="checkbox"/>     |                                                                                      |
| 创建时间:                                       | Dec 14, 2020, 9:02 AM, CST              |                                                                                      |
| 到期日:                                        | <input type="text" value="12-31-2020"/> | (月份-日期-年份 (mm-dd-yyyy) )                                                             |
| 到期时间:                                       | <input type="text" value="12:00"/>      | (小时: 分钟, 24 小时制 (hh:mm) )                                                            |
| 在截止日期之后记录所有学生的作业?                           | <input type="checkbox"/>                | 如果未选中此复选框, 则 ACE 将强制执行截止日期, 并且不会将任何在截止日期之后完成的作业记录在成绩册中, 如果您希望随时间变化的分级参数生效, 请选中此框。    |
| 这个任务是计时考试吗?                                 | <input type="checkbox"/>                | 如果选中此框, 则延长期限和过期时间将以分钟 (而不是天) 为单位计算, 在学生提交回答时, ACE 每次都会检查过期日期和时间, 而不仅仅是在显示作业列表页面时显示。 |
| 这个任务是计时考试吗?                                 | <input type="checkbox"/>                |                                                                                      |
| 延迟评分?                                       | <input type="checkbox"/>                | 如果选中此框, 则仅在您按下成绩册中的 "重新评分" 按钮后, ACE 才会对学生的回答进行评分并提供反馈。                               |
| 从课程中移除任务?                                   | <input type="checkbox"/>                | 如果选中此框, ACE 将从课程成绩总分中扣除此作业的成绩。                                                       |
| 对学生显示参考文献 (哪里可获取)?                          | <input type="text" value="从不"/>         | 试题的作者可以在试题创作工具中输入参考文献。                                                               |
| 写出数据库中的每一个回答?                               | <input type="checkbox"/>                | 如果选中此框, 则新的回答不会覆盖数据库中先前的回答, 并且您将在成绩册中看到先前的回答。                                        |
| 每个回答都保存到本地计算机?                              | <input type="checkbox"/>                | 如果选中此框, ACE 将以您可以在浏览器中查看的格式将每个回答记录到磁盘。                                               |
| 提交之前, 允许保存?                                 | <input type="checkbox"/>                | 如果选中此框, ACE 将允许学生保存作业, 而无需将其提交评分, 直到准备就绪。当采用尝试次数相关的评分时, 此选项很有用。                      |
| <b>尝试次数相关的评分</b>                            |                                         | 随着尝试次数的增加逐渐降低学生的作业成绩, 被调整的分只显示在成绩册中。                                                 |
| <a href="#">增加评分参数</a>                      |                                         |                                                                                      |
| <b>学习时间相关的评分</b>                            |                                         | 自过期时间开始随天数增加逐渐降低学生作业的成绩。仅根据成绩册中的显示来调整成绩。                                             |
| <a href="#">增加评分参数</a>                      |                                         |                                                                                      |
| <b>延长期限</b>                                 |                                         |                                                                                      |
| <input type="text" value="自行允许的最长延期时限: v"/> |                                         | <input type="text" value="3"/> 天                                                     |
| <a href="#">对个别学生延长期限</a>                   |                                         |                                                                                      |
| 您没有准予延长期限。                                  |                                         |                                                                                      |

提交

取消

Fig. 3. The teacher editing task parameter interface in ACE

After students complete the exercises, ACE will grade them according to the teacher's scoring rules. Teachers can see each student's score through the website's statistics, and can also view each student's final answer to each exercise through the link. Detailed statistical data not only helps teachers understand the overall learning situation of students, but also helps teachers find problems with individual students.

### 1.3 Author tools

In order to meet the personalized needs of teachers for exercises, ACE has a special author tool. Teachers can edit existing exercises or create new exercises according to the teaching content. The author tool of ACE is slightly complicated. Editing or creating new exercises includes three parts: editing the question stem, drawing the molecular structure, etc. (reaction questions need to draw the reactants and reaction conditions, mechanism questions need to draw the reaction formula, synthesis questions need to draw the structure of the target molecule, etc.), and giving feedback on the answers (Fig. 4). The more complicated part is editing feedback on different answers. As shown in Fig. 5, it is necessary to classify the possible answers of students into different situations (correct, partially correct, wrong). First, for the correct answer, the knowledge points involved in the exercise should be prompted, and the solution ideas should be proposed. Secondly, it is necessary to preset a variety of incompletely correct or wrong answers that students may give, and propose the reasons for the mistakes for each answer, and guide students to think about the problem scientifically. In addition, if the answer submitted by the student is not within the preset range, the teacher can add corresponding feedback information items according to the situation.

The screenshot displays the ACE Organic Author interface. At the top is a navigation bar with links: My Courses, My Profile, Question Bank, Textbooks, Crosscourse reports, and Logout. The main area is divided into several sections:

- Question type:** A dropdown menu currently set to "Skeletal structure".
- Question properties:** A group of checkboxes including "uses R groups", "don't highlight valence errors", "put coordinate bond button on toolbar", "disallow unnecessary wedge bonds", "show lone pairs", "show mapping", "uses 3D conformations", and "show R,S labels".
- Marvin initialization parameters:** A group of checkboxes including "preload figure", "show explicit H atoms only", and "show R,S labels".
- Question source:** Fields for "Book:" (dropdown), "Author:" (text input with "RBG"), and "Number:" (text input with "[None]").
- Keywords:** A text input field containing "RBG Acidity and basicity Rank the strongest/weakest acid/ba..".
- New Question Statement:** A large empty text area for the question stem.
- Figures:** A section with a "[None]" label and an "Add New" button.
- Evaluators:** A section with an "Add New" button and a "View functional groups" button.

At the bottom of the interface is a row of action buttons: Preview, Save, Save and Add New, Save and Duplicate, Save and Exit, and Cancel.

Fig. 4. Author interface in ACE

**New:** Wrong ▾

If the number of atoms of an element ▾

If the response has ▾

a total number of ▾

C atoms that is not exactly ▾ 0

You may specify a particular isotope of an element (e.g., "D" or "<sup>13</sup>C"). If you do not specify a particular isotope, ACE will count all isotopes of the element toward the total. ACE will count implicit H atoms toward the total if you enter "H" but not if you enter "<sup>1</sup>H". Use "X" to count every atom.

**Feedback** (Leave blank if this evaluator is or will be part of a compound evaluator)

Save, close Save, add new Save, add clone Cancel

Fig. 5. Editing feedback interface in ACE

## 2. Application of ACE in organic chemistry teaching

The School of Chemistry at Jilin University offers a two-semester basic organic chemistry course for sophomores, with nearly 300 students in each grade. In the first half of 2020, during the COVID-19 pandemic, the teaching team began to try to assign exercises in ACE to replace some paper homework. Compared with written homework, ACE has a real-time feedback function, which greatly improves students' learning efficiency. After using ACE, students gave good feedback: they mastered the skills of drawing organic structures on the computer through ACE; the real-time feedback of the system could solve most of the problems in the exercises; the ACE forum provided convenience for teachers and students to discuss problems in depth; and the interest in learning organic chemistry was

increased. In the teaching cycle of organic chemistry using ACE, students were more receptive to online homework (Fig. 6).

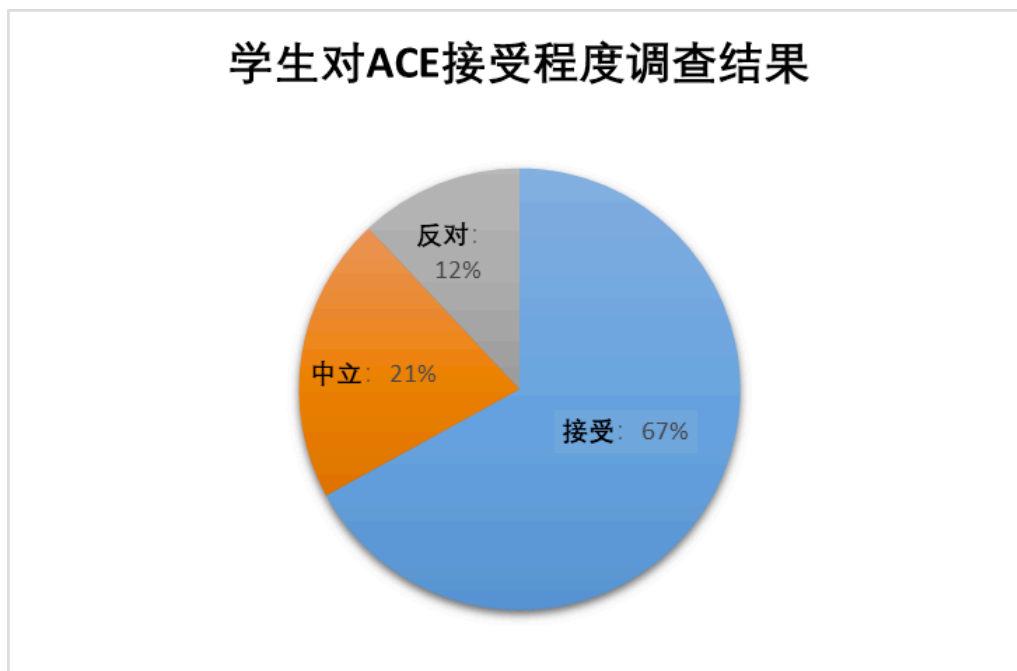


Fig. 6. Results of a survey on students' acceptance of ACE. [Blue indicates acceptance, gray indicates opposition.]

### 3. Conclusion

ACE: Organic Chemistry is a relatively complete and powerful online organic chemistry problem platform based on the web. The system is highly intelligent and can comment on the answers submitted by students in real time. It can not only judge whether the answers are correct or not, but also give the reasons for correctness and errors. Compared with traditional paper homework, it can stimulate students' learning interest and enthusiasm for independent learning, improve their learning efficiency and independent thinking ability, broaden their horizons, and enhance students' adaptability to society. In addition, the statistical data provided by ACE can help teachers grasp students' learning situation more comprehensively and systematically, and the time saved from reviewing homework can be used to interact with students to achieve better teaching results.

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