



Virtual laboratory



SCIENCE

Organic chemistry

User
manual



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Terms and Definitions

The following general terms are used in the User Guide:

Virtual laboratory	Virtual Laboratory "Science", "Organic Chemistry" section
Scene	A virtual three-dimensional space within which the user can interact with the Virtual laboratory objects. The concept of "scene" also includes the data of the current research (positions of objects, their parameters, etc.)
Camera	A scene tool with which the user observes everything that happens in the Virtual laboratory.
Click	To make a click: — when using a mouse, move the mouse pointer to the object, press and release the left mouse button without moving the pointer; — when using a touchscreen, press the object with a finger and release it without moving the finger along the screen.
Toggle-button	A button that changes its state from inactive to active and vice versa after being pressed. The state is retained until the next interaction.

1 System requirements

Minimum system requirements for the Virtual Laboratory "Science", "Organic Chemistry" section are:

- **Processor:** Intel Ivy Bridge series / AMD Bulldozer series.
- **RAM:** 4 GB.
- Graphics Card:
 - Integrated: Intel HD Graphics 5000 / Intel;
 - Discrete: GeForce 400 series / Radeon HD 7000 series.
- **Screen Resolution:** 1920x1080 / 1920x1200 (4K and Retina displays require a more powerful graphics card for comfortable operation).
- **Supported Browsers:** Chrome, Yandex.Browser, Opera 44+, Firefox 51+, Edge 79+, Safari 15+.
- **Supported Operating Systems:**
 - Microsoft Windows 7 (x64 versions) with WebGL 2.0 driver support;
 - MacOS X "Snow Leopard" 10.6 with WebGL 2.0 driver support;
 - Linux or Debian with WebGL 2.0 driver support.

2 Virtual laboratory interface

The Virtual Laboratory interface (Figure 1) includes the following elements:

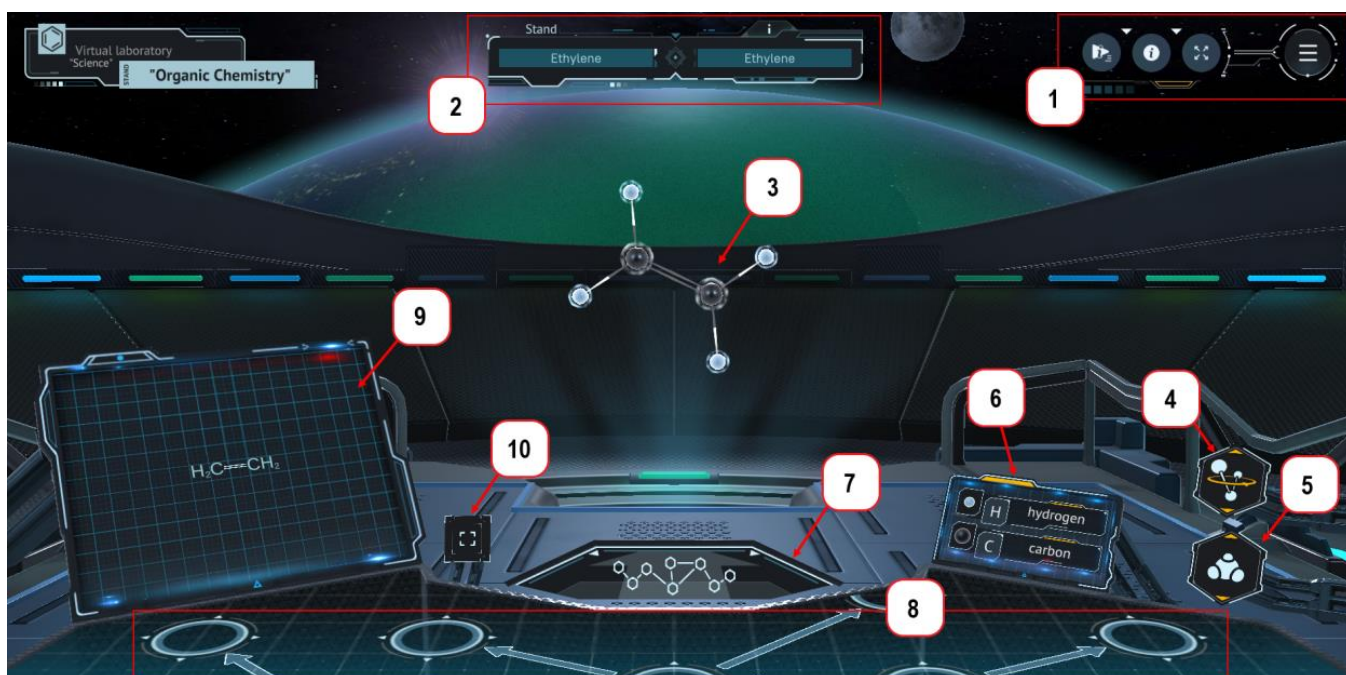


Figure 1 – Virtual Laboratory "Science", "Organic Chemistry"

- 1) **Main menu** (see [4 Main menu](#)).
- 2) **Stand control panel** (see [5.1 Stand control panel](#))
- 3) **Molecule model** (see [5.2 Molecule model](#)).
- 4) **Start/stop rotation button** (see [5.2 Molecule model](#)).
- 5) **Molecule model type selector** (see [5.2 Molecule model](#)).
- 6) **Legend display** (see [5.2 Molecule model](#)).
- 7) **Show reaction chain button** (see [5.3 Reaction chains](#)).
- 8) **Reaction chain display** (see [5.3 Reaction chains](#)).
- 9) **Information display** (see [5.2 Molecule model](#)).
- 10) **Info display zoom button** (see [5.2 Molecule model](#)).

3 Camera control

The camera is controlled using the mouse or your fingers (when working with a touch screen).

While the application is loading, the camera is in default position — focused at the center of the table (Figure 1).

To zoom in/out, rotate the mouse wheel. When using the touch screen, touch the screen with two fingers, spreading them apart or pressing them together.

To move the camera, hold down the right mouse button anywhere in the scene; drag the pointer in the desired direction and then release it. Camera movement is available only if the molecule model goes outside the screen (Figure 2).

To focus the camera on the installation, click on  button at the bottom of the screen (Figure 2).

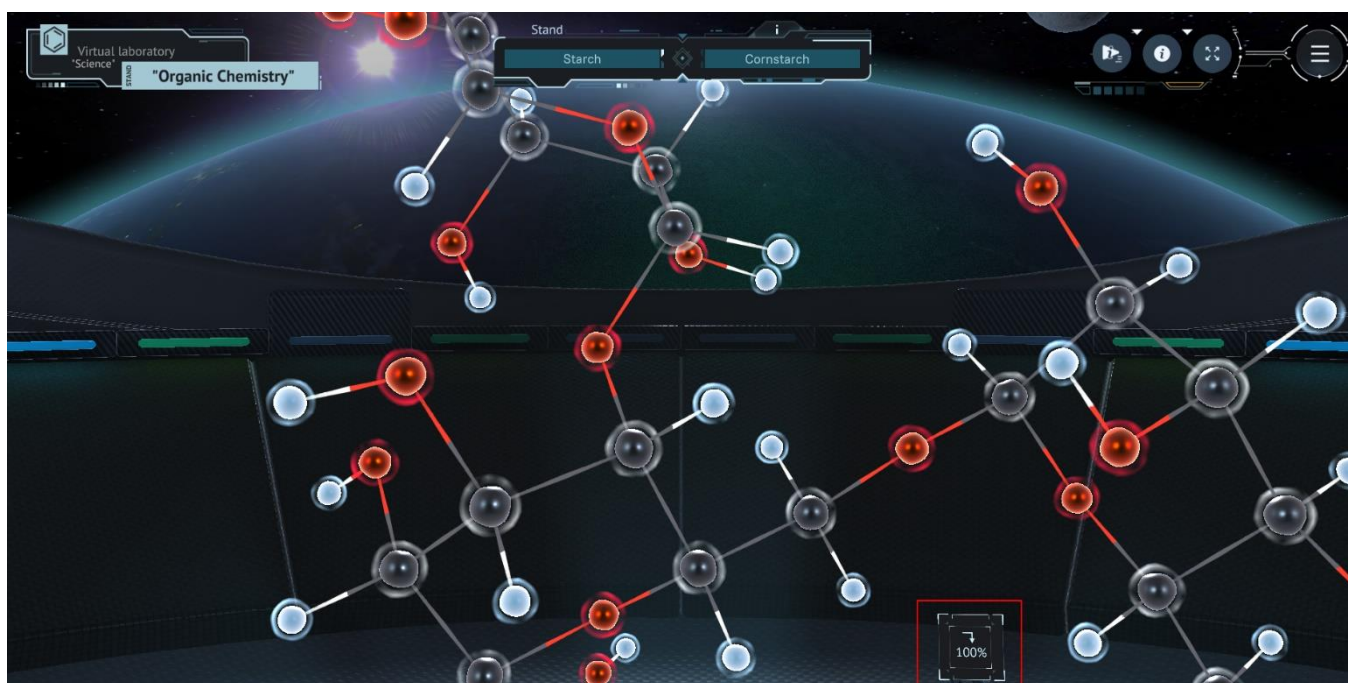


Figure 2 – Molecule model beyond the screen

4 Main menu

The main menu is located in the upper right corner of the app (1 in Figure 1) and consists of the following elements (Figure 3):

- **Instructions** button  (see [4.1 Instructions](#));
- **Tips mode** button  (see [4.2 Tips mode](#));
- **Fullscreen mode** button  (see [4.3 Fullscreen mode](#)).
- **Scene menu** button  (see [4.4 Scene menu](#)).



Figure 3 – Main menu

4.1 Instructions

To select an instruction to view, click the **Instructions**  toggle-button in the **Main menu** (Figure 3). An instruction selection menu will open (Figure 4). Read **User Manual** or watch video instructions to learn:

- how to work with the scene and equipment — "Introduction video";
- how to save created scenes and load saved scenes — "Saving and loading".

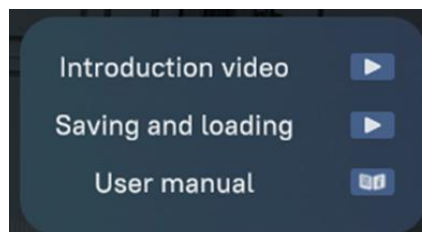


Figure 4 – Menu for selecting instructions

Click on the video title to start watching. The video will play on the screen over the scene. Control playback using the built-in player (Figure 5).

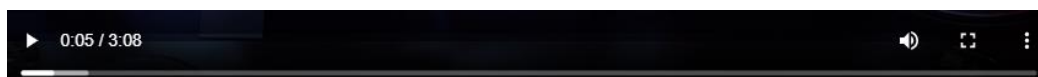


Figure 5 –Player control elements

To close the playback screen, click the **Close** button  in the top right corner of the screen.

To close the video instructions selection menu, press the  button.

4.2 Tips mode

To switch to the interactive tips mode, click the **Tips mode** toggle-button  in the **Main menu** (Figure 3). Tips points will appear next to the objects in the scene (Figure 6).



Figure 6 – Tips mode

To view a tip, press the point. To close the tip panel, press the tip point again or click on the cross in the upper right corner of the panel.

Tip points change their outline color depending on whether the user has viewed the tip or not (Figure 7):

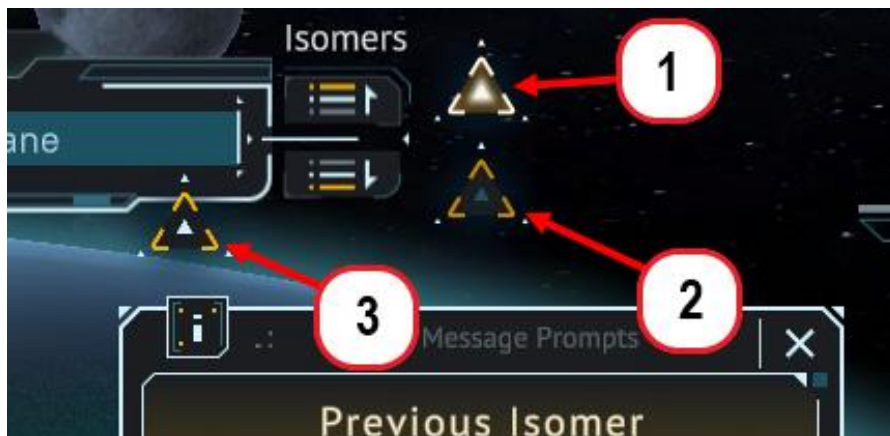


Figure 7 – Point outline color options

- 1) Button with illuminated center  — the tip is open on the screen.
- 2) Button with grey center  — the user previously viewed and closed the tip.
- 3) Button with white center  — the user has not yet viewed this tip.

In addition, at the top of the scene there is an icon for a tip on how to interact with the molecule model (Figure 8).



Figure 8 – Icon for a tip on molecule model interaction

To exit the **Tips mode**, press the  button in the **Main menu**.

4.3 Fullscreen mode

To enable full screen mode, press the **Fullscreen Mode** button  in the **Main menu** (Figure 3). The application will expand to full screen, hiding the browser frame and the OS taskbar. To exit full screen mode, press the  button or the **Esc** button on your keyboard.

4.4 Scene menu

Working in the Virtual laboratory, you can:

- save the current scene (see [4.4.1 Saving a scene](#));
- save the copy of the current scene (see [4.4.2 Saving a copy of a scene](#));
- create a new scene (see [4.4.3 Creating a new scene](#));
- open the **My scenes** library (see [4.4.4 Viewing and loading user scenes](#)).

To go to one of the actions, click the  button in the **Main menu** (Figure 3) and select the desired menu item for working with the scenes (Figure 9). A line with the user's name appears above the menu.

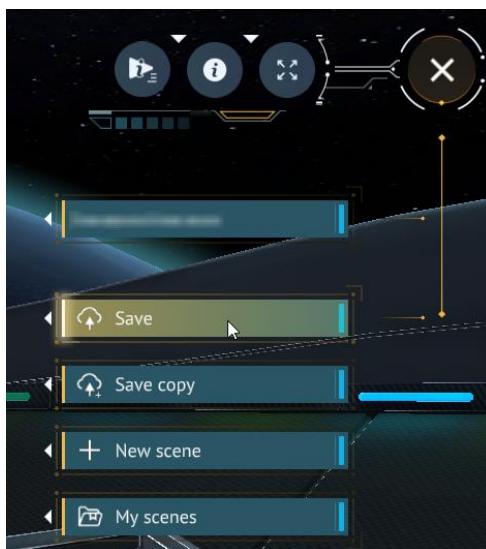


Figure 9 – Scene menu

To close the **Scene menu** and the **Main menu**, press the  button or click anywhere in the scene outside the menu.

4.4.1 Saving a scene

To save the created scene in the **My scenes** library, select **Save** in the **Scene menu** (Figure 9).

If the scene has already been saved, the application will overwrite the contents of the scene file. If the scene is being saved for the first time, the save scene form will open (Figure 10).

Figure 10 – Scene saving form

The **Creator** line displays the name of the scene creator. If the scene was modified by another user, an **Editor** line with their name will appear under the **Creator** line.

Enter the **name of the scene** to be saved (no more than 36 characters) and its **description** (no more than 1000 characters) in the appropriate fields of the form and click the **Save** button.

You can use the virtual keyboard if necessary. To do so, use the  button, located to the left of the saving form.

If you want to cancel the saving of the scene, press the **Cancel** button.

4.4.2 Saving a copy of a scene

To save a copy of the scene in the **My Scenes** library, select **Save copy** in the **Scene menu** (Figure 9). This will open the form for saving a copy of the scene, which is similar to the scene saving form (Figure 10).

If the scene is being saved for the first time, you must fill in the **Scene name** (no more than 36 characters) and **Scene description** (no more than 1000 characters) fields.

If the scene has already been saved, the previously saved scene name with the copy number in brackets will be displayed in the **Scene name** field — **Scene 1(2)**. The scene name and copy number can be adjusted or left unchanged.

Click the **Save** button to save a copy of the scene.

After you have saved a copy, you will continue to work with it, and the copy of the scene you worked with before will remain in the state of its last save.

If you do not need to save the scene copy, press the **Cancel** button.

4.4.3 Creating a new scene

To create a new scene, select **New scene** in the **Scene menu** (Figure 9). If there are unsaved data, a window with a warning about possible data loss (Figure 11) will open.



Figure 11 – Create new scene window

To avoid losing the current data, click the  button and continue working with the scene. If you do not need to save the data, click the  button, after which all unsaved data will be lost and a new empty scene will open.

4.4.4 Viewing and loading user scenes

To view a list of scenes, select **My scenes** in the **Scene menu** (Figure 9). **My Scenes** library page (Figure 12) will open.

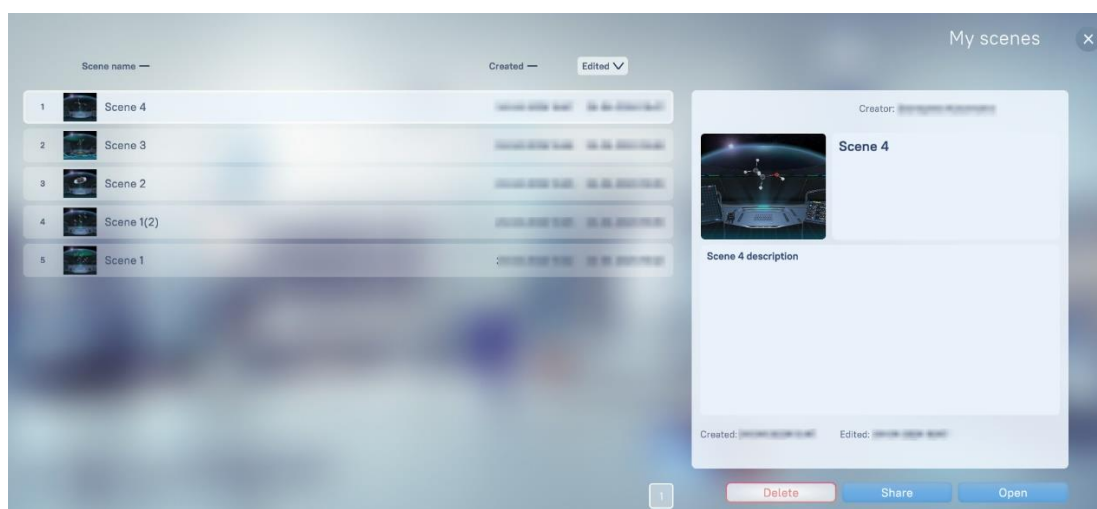


Figure 12 – My scenes library

On the left side of the screen, a list of all saved scenes will be displayed. You can sort the data by scene name, creation date, and modification date. To sort, click on the name of the corresponding table column (Name, Created or Modified). The  icon next to the name will change to a check mark, indicating

the sorting direction .

If the list of scenes does not fit on one screen, it will be split into pages. Navigation through the pages is done using a series of buttons with page numbers, located to the right under the table.

The information about the selected scene is in the scene card to the right of the table. If necessary, you can open, delete, or share the selected scene using the buttons located under the scene card.

5 Objects description

5.1 Stand control panel

Stand control panel (2 in Figure 1) is located at the top of the screen and consists of the following elements (Figure 13):

- 1) **stand selection** button;
- 2) **isomer selection** button;
- 3) **methodological information** button.



Figure 13 – Stand control panel

Each stand demonstrates one model of a molecule. The name of the current stand is displayed on the button (1). To switch to another stand, press the button (1) and select the desired stand in the opening list (Figure 14). All stands work independently from each other. To close the list of stands, click again on the button (1) or anywhere on the scene outside the list.

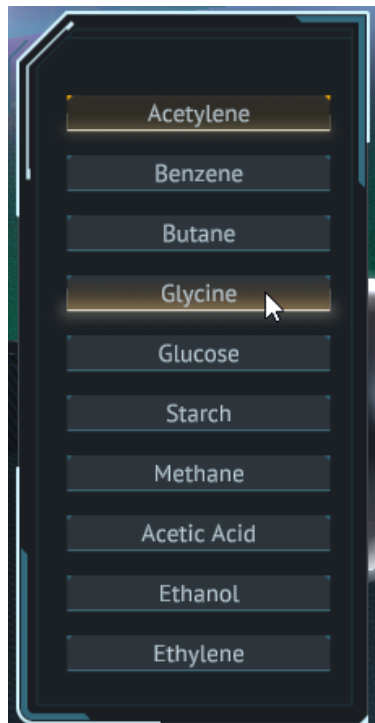


Figure 14 – Stand list



Figure 15 – Isomer stands switching buttons



Figure 16 – Isomer list

For some substances (butane, glycine, glucose) additional stands with isomers are available. During operation of a stand for which stands with isomers are available, buttons for switching isomer stands are displayed to the right of the control panel (Figure 15).

To switch to the stand of the desired isomer, press the button (2) in Figure 17 and select the desired stand in the list that opens (Figure 16). You can also switch between stands by pressing the  and  buttons to the right of the control panel.

To return to the main substance stand, press the  button (Figure 18).



Figure 18 – Button to go to the main substance stand

To open a card with methodological information, click the  button (3 in Figure 13). The card will open in the center of the scene. (Figure 19). To scroll through the information on a card, hover your mouse over it, roll your mouse wheel or drag the scroll bar at the right edge of the card.

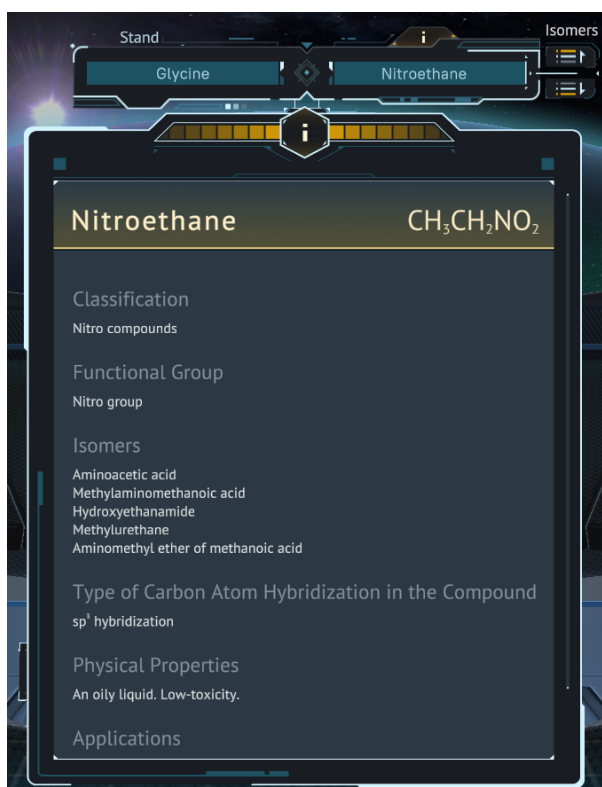


Figure 19 – Card with methodological information

To close the methodological information, press the  button again or click anywhere in the scene outside the card.

5.2 Molecule model

A ball-and-stick model of a substance molecule is displayed in the center of the scene (3 in Figure 1). The ball-and-stick model shows the structure of the molecule of organic substances, the direction of chemical bonds and the values of valence angles (Figure 20).

Molecule model type can be changed: click the  button (5 in Figure 1), to enable display of the hemispherical model of the molecule. The hemispherical model represents real molecules, considering the arrangement of atoms, interatomic distances and atomic sizes (Figure 21). To return to the ball-and-stick model, click the  button.



Figure 20 – Ball-and-stick model of the butane molecule

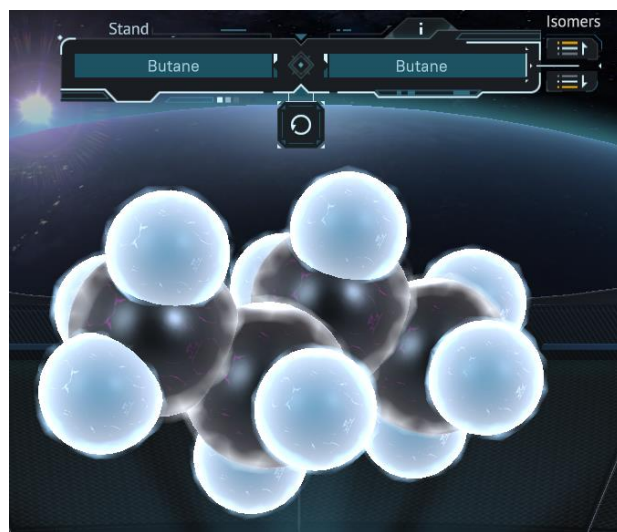


Figure 21 – Hemispherical model of the butane molecule

To zoom in/out on the model, rotate the mouse wheel or pinch/spread your fingers on the touch screen. If the model extends off the screen, move the camera to view the desired part of the model. To do this, hold down the right mouse button in any free place in the scene, drag the pointer in any direction to the desired camera position and release it.

By default, the molecule model rotates automatically. To rotate the model manually, hold down the left mouse button, drag the pointer in any direction to the desired position of the model, and then release it.

To stop the model from rotating, press the  button (4 in Figure 1) — the button will change to , the molecule model will stop rotating. To turn rotation back on, press the  button.

The **Legend** display (6 in Figure 1) displays the composition of the molecule: color and letter designations of atoms and their names (Figure 22). The order of atoms in the list depends on their number in the substance: the more atoms, the higher the substance in the list. When the number of atoms is the same, substances are sorted by the element's serial number in the periodic table of chemical elements in increasing order.

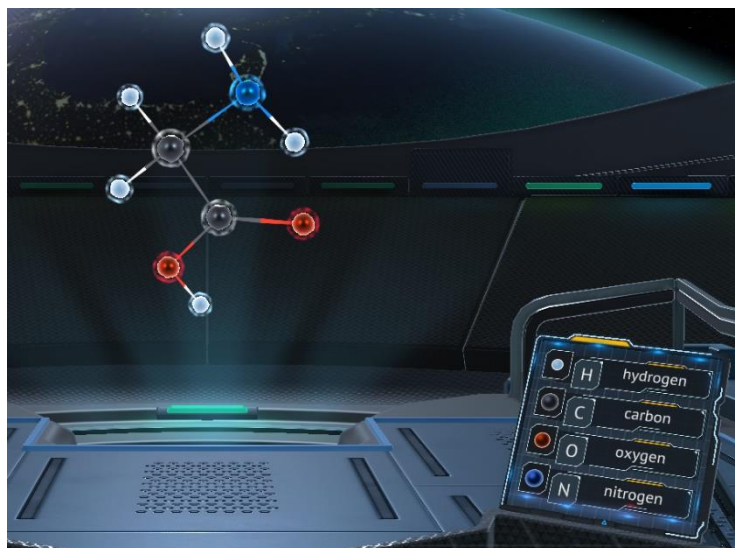


Figure 22 – Displaying the composition of a molecule on the Legend display

Reaction chain diagrams are available for benzene and ethylene molecules. Click the  button (7 in Figure 1) and information about the transformations of the substance will be displayed on the **Chain reaction** display (8 in Figure 1). For more about reaction chains, see [5.3 Reaction chains](#).

In the **Information display** (9 in Figure 1) the structural formula of the substance is displayed (Figure 23). It can also show transition conditions in a reaction chain (Figure 24).

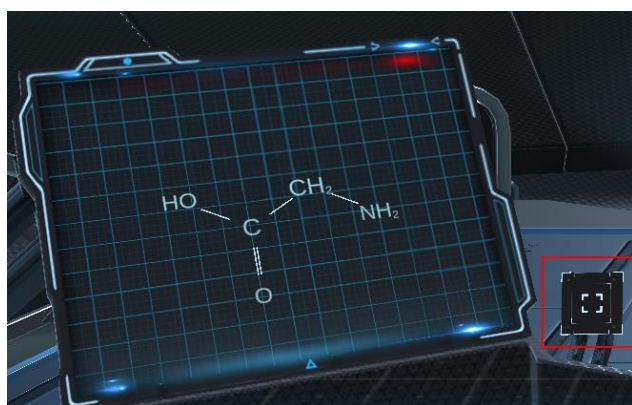


Figure 23 – Structural formula of a substance on the information display

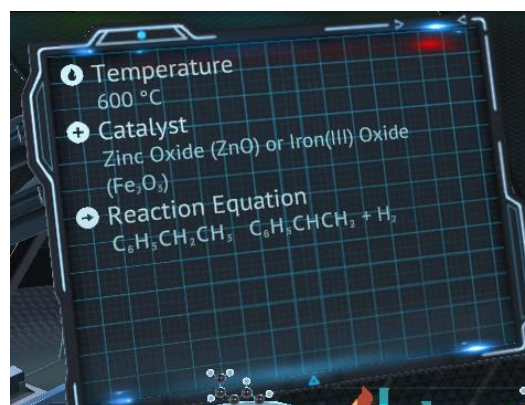


Figure 24 – Transition conditions in the chain of reactions

To see the display in fullscreen mode (Figure 25) press the  button (10 in Figure 1). To return the screen to its default position, press the  button.

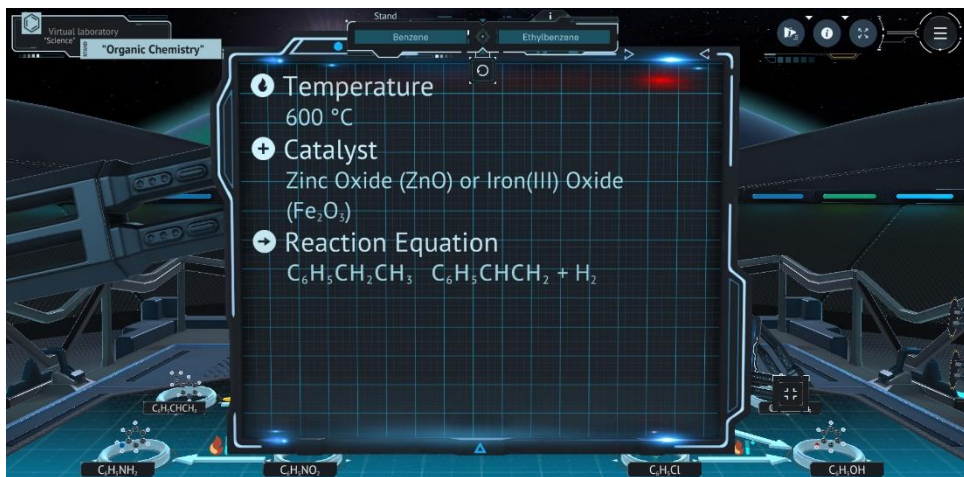


Figure 25 – Expanded information display

5.3 Reaction chains

Reaction chains are available for benzene and ethylene molecules. Click the  button (7 in Figure 1) and information about substance transformations (Figure 26) will be displayed on **Reaction chains** display (8 in Figure 1).



Figure 26 – Reaction chain display

Above each button of a substance is a model of its molecule, and below the button is a chemical formula. The structural formula of the selected compound is shown on the information display. By default, the main substance of the stand is selected, its button is colored yellow. To select another substance, click on the corresponding button - the button will change color from blue to yellow, the molecule model and structural formula will change.

The arrows between the buttons indicate the direction of the reaction between substances:

- one arrow — the reaction is irreversible;
- two arrows — the reaction is reversible.

Above the arrows there are buttons indicating the reaction conditions:

- heating ;
- reagent adding ;
- heating and reagent adding ;
- heating and reagent adding and additional impact (for example, pressure) .

To view detailed information about the reaction conditions and its equation, click on the button above the arrow — the reaction arrow will change its color to yellow; the data will be displayed on the Information display (Figure 27).

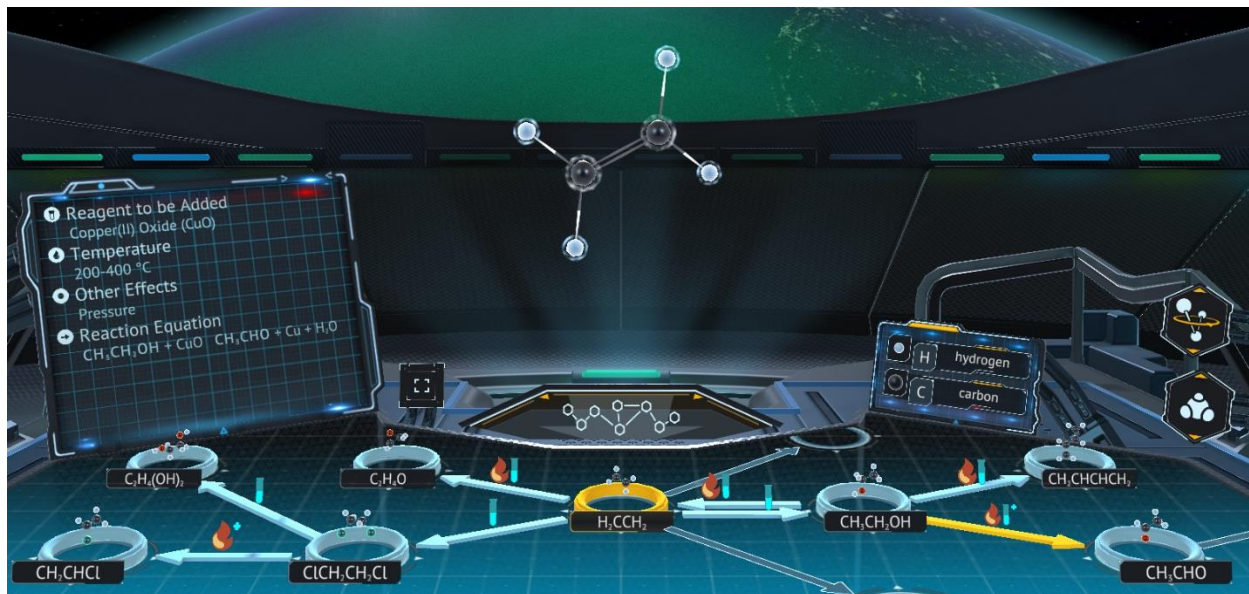


Figure 27 – Information about reaction conditions on the display

To return to the structural formula of a substance on the information display, press the button for the desired substance or press the button above the arrow again.