INDIVIDUAL TASK
«VISUALIZATION OF A MOLECULE»

FORMULATION OF THE TASK

It is required to develop a program that visualizes the structure of the molecule of the substance indicated in the variant of an individual assignment according to Table 1. The visualization scheme should to some extent correspond to the image shown in Fig. 1, identical atoms should be represented by balls of the same color, atoms of different elements – by balls of different colors. The bonds between atoms should be represented by sufficiently thin cylinders, with one cylinder corresponding to a single bond, and two, respectively, to a double bond. The color of the cylinders depicting a bond should correspond to the colors of the atoms connected by it; if the atoms are different, the cylinder should be two-colored. The type of coloring of such a cylinder – an abrupt color transition or mixing of colors – is indicated in Table 1. The name of the substance and its chemical formula should be presented above the window with the image of the molecule.

The ability to enable / disable labels denoting the name of the atom should be implemented as an interface element. The location of the label in relation to the image of the atom must correspond to the variant from Table 2.

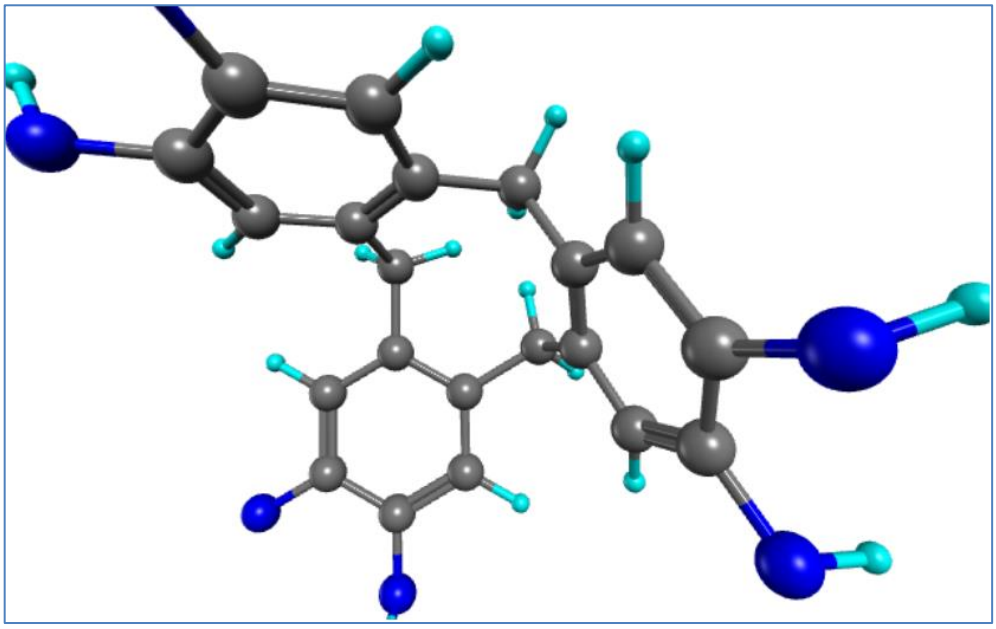


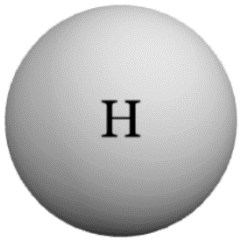
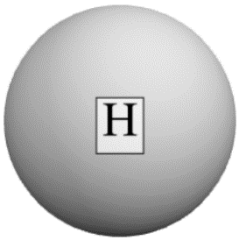
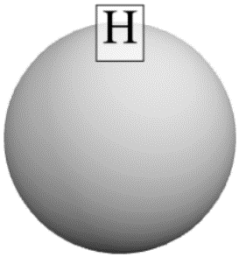
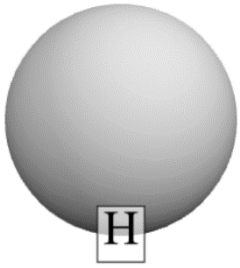
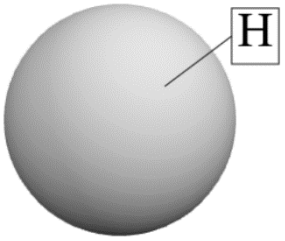
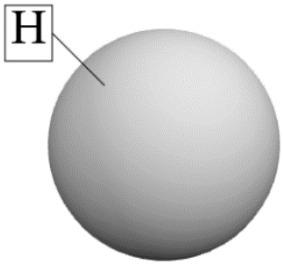
Fig. 1. Approximate expected result of visualization

Table 1. Variants of an individual assignment

Option number	Substance name, chemical formula	Label arrangement option	Staining type
1	Cholesterol, $C_{27}H_{46}O$	А	Abrupt transition
2	Alpha-eucaine, $C_{19}H_{27}NO_4$	Б	Color mixing
3	2-methylpropyl 4-phenylbutanoate, $C_{14}H_{20}O_2$	В	Abrupt transition
4	2,3-Diphenylquinoxaline, $C_{20}H_{14}N_2$	Г	Color mixing
5	Bromopride, $C_{14}H_{22}BrN_3O_2$	Д	Abrupt transition
6	6-Benzoyl-2-naphthol, $C_{17}H_{12}O_2$	Е	Color mixing
7	Aequinetin, $C_{21}H_{20}O_9$	А	Abrupt transition
8	Trp-AFC, $C_{21}H_{16}F_3N_3O_3$	Б	Color mixing
9	Sempervilam, $C_{19}H_{16}N_2$	В	Abrupt transition
10	Decyl hydrogen phthalate, $C_{18}H_{26}O_4$	Г	Color mixing
11	Hexaphenol, $C_{21}H_{18}O_6$	Д	Abrupt transition
12	Cyclenar, $C_{15}H_{27}N_5$	Е	Color mixing
13	Lamotrigine, $C_9H_7Cl_2N_5$	А	Abrupt transition
14	Andrograpanin acetate, $C_{22}H_{32}O_4$	Б	Color mixing
15	ROSIN, $C_{15}H_{20}O_6$	В	Abrupt transition
16	Cannabifuran, $C_{21}H_{26}O_2$	Г	Color mixing
17	Sorgomol, $C_{19}H_{22}O_6$	Д	Abrupt transition
18	Hemistepsin, $C_{19}H_{22}O_6$	Е	Color mixing
19	Asperinin A, $C_{32}H_{26}O_{10}$	А	Abrupt transition
20	7281P, $C_{40}H_{44}O_6$	Б	Color mixing
21	AMINOPYRINE, $C_{13}H_{17}N_3O$	В	Abrupt transition
22	Melatonin, $C_{13}H_{16}N_2O_2$	Г	Color mixing

23	Cortisone, $C_{21}H_{28}O_5$	Д	Abrupt transition
24	Hexahelicene, $C_{26}H_{16}$	Е	Color mixing

Table 1. Label arrangement options

 Option А	 Option Б	 Option В
 Option Г	 Option Д	 Option Е

INSTRUCTIONS FOR COMPLETING THE TASK

To build a model, first of all, you need data on the coordinates of its atoms, that is, a file in one of the formats used in chemical informatics. To search for such a file, we will use the Mol-Instincts database of chemical compounds. All chemical compounds presented in Table 1 are freely available in this database.

To search for the structure file, you can use the search form on the website www.molinstincts.com, or you can search using the usual Google search engine by entering the following text in the search bar:

```
ethylene mol file Mol-Instincts
```

In this query, ethylene is the name of the substance you are looking for, mol is the file format we hope to find. The search results are shown in Fig. 2. It can be seen that the first two links are likely to provide the required data.

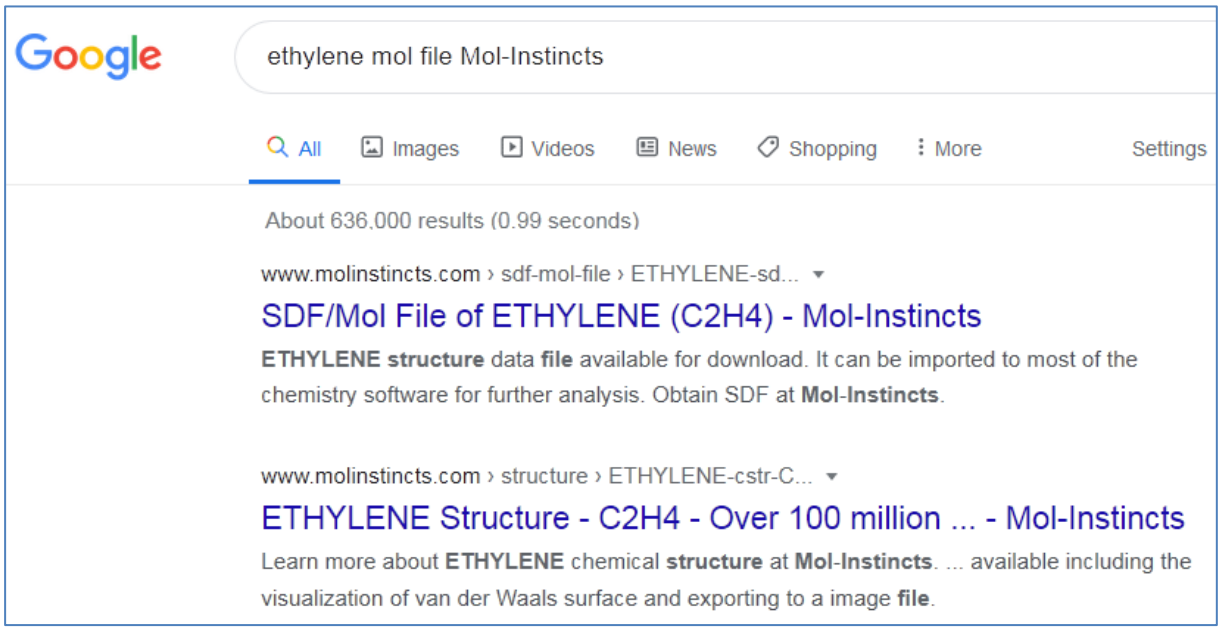
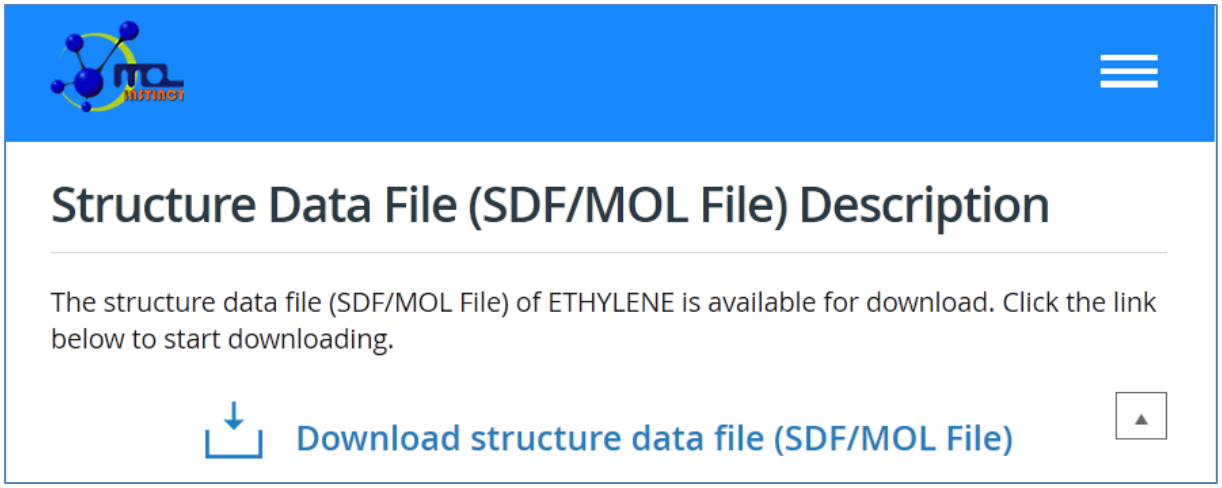
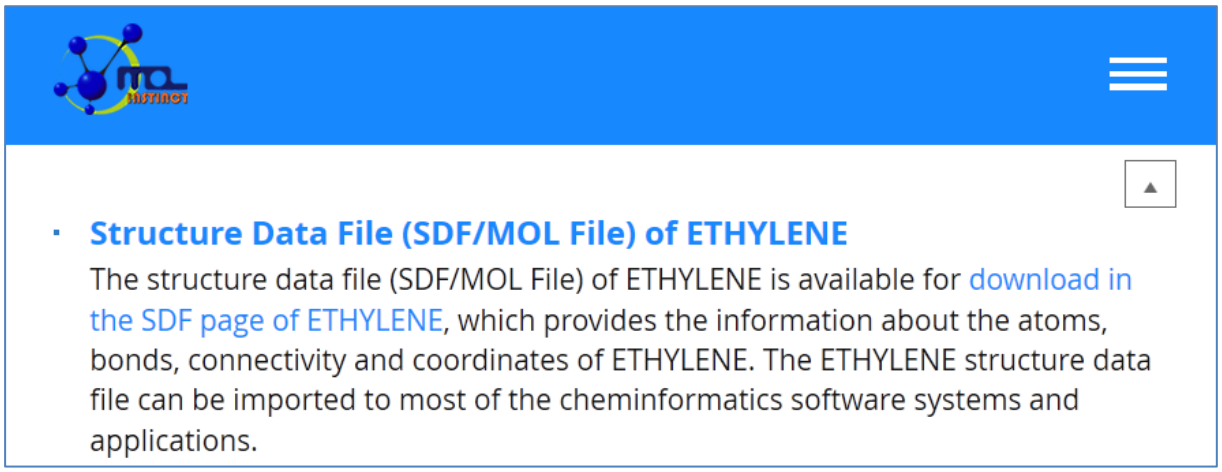


Fig. 1. File with molecule structure data search results

Depending on the link you choose, you can get to slightly different pages of the ethylene database. In the first case, the link to download the file immediately catches the eye:



In the second case, this link is in the middle of the page, after the description of the chemical structure and the list of properties, in the **Additional Information** section, and looks something like this:



- **Structure Data File (SDF/MOL File) of ETHYLENE**

  The structure data file (SDF/MOL File) of ETHYLENE is available for download in the SDF page of ETHYLENE, which provides the information about the atoms, bonds, connectivity and coordinates of ETHYLENE. The ETHYLENE structure data file can be imported to most of the cheminformatics software systems and applications.

Pay attention to the abbreviation SDF/MOL. The structure of these files is practically identical, if they store information not about several substances at once, but only about one, as in this case.

The downloaded file is named ETHYLENE-3D-structure-CT1002310794.sdf. For the convenience of further work, let's rename it to ethylene.sdf. Having opened the downloaded file in any text editor (it is quite possible to get by with the standard Notepad application), we make sure that this is really a file of the required structure.

```
1  CT1002310794
2
3
4    6  5  0  0  0               999 V2000
5     -0.0126    1.0758    0.0080 C   0  0  0  0  0  0  0  0  0  0  0  0
6      0.0021   -0.0041    0.0020 H   0  0  0  0  0  0  0  0  0  0  0  0
7      0.9153    1.6285    0.0021 H   0  0  0  0  0  0  0  0  0  0  0  0
8     -1.1558    1.7153    0.0169 C   0  0  0  0  0  0  0  0  0  0  0  0
9     -1.1705    2.7952    0.0228 H   0  0  0  0  0  0  0  0  0  0  0  0
10    -2.0837    1.1627    0.0183 H   0  0  0  0  0  0  0  0  0  0  0  0
11   1  2  1  0  0  0  0
12   1  3  1  0  0  0  0
13   1  4  2  0  0  0  0
14   4  5  1  0  0  0  0
15   4  6  1  0  0  0  0
16 M  END
17 $$$$
```