

REACK

Balancing and calculations on chemical equations

The screenshot shows the REACK software window titled "Chemical equations: balancing and calculations". The window has a menu bar with "File", "Data", "Tools", "Info", and "Exit". Below the menu bar, there is a "Reaction" input field containing the chemical equation $C_4H_{10} + O_2 \longrightarrow CO_2 + H_2O$. To the right of the input field are three buttons: "New", "Balance", and "AutoBalance". Below the input field, there is a section titled "Reactants / Products" which is divided into two columns: "Reactants" and "Products". The "Reactants" column contains a list of chemical formulas: "C4H10" and "O2". To the right of this list are three empty input fields labeled "Initial", "mol r.", and "end". The "Products" column contains a list of chemical formulas: "CO2" and "H2O". To the right of this list is one empty input field labeled "mol". Below the "Reactants" and "Products" sections, there are two yellow input fields, each with an upward arrow button. Between these two yellow input fields are two buttons: "+" and "-".

- [Reactions: importing and editing](#)
- [Balancing a reaction](#)
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Reactions: importing and editing

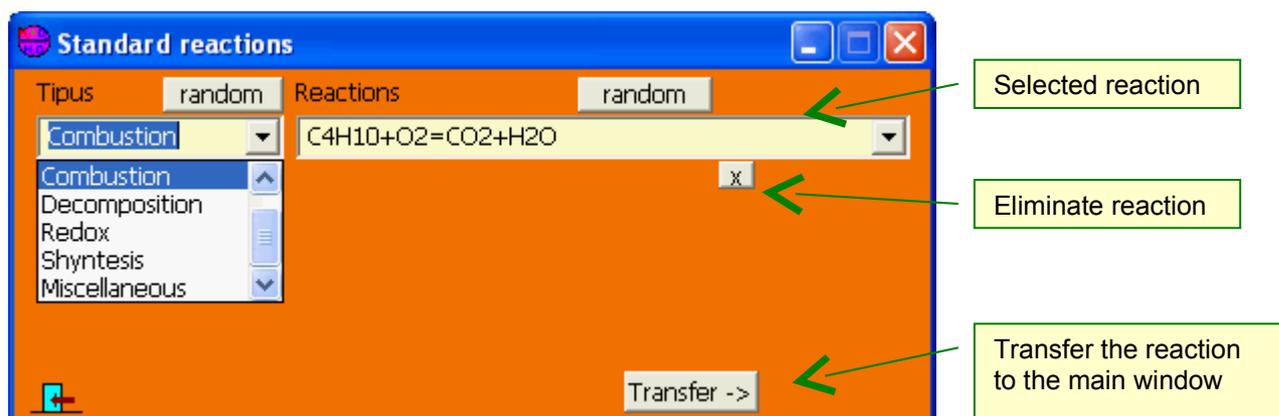
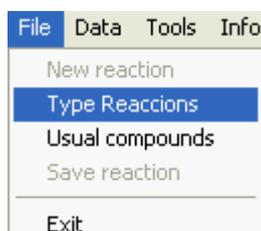
Only are supported “molecular” (not ionic) reactions, and they only may consist in formulas and coefficients (not other indications)

- [Importing standard reactions](#)
- [Building /editing manually a chemical equation](#)

Importing standard reactions

Clicking on the menu **File** option...

The window that connects with the database of standard reactions is shown

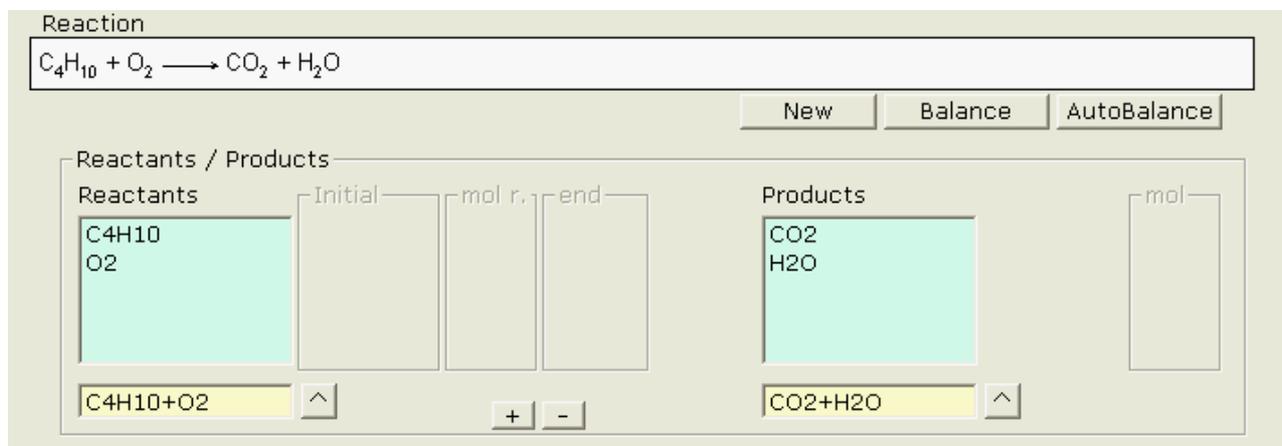


At this window you can also:

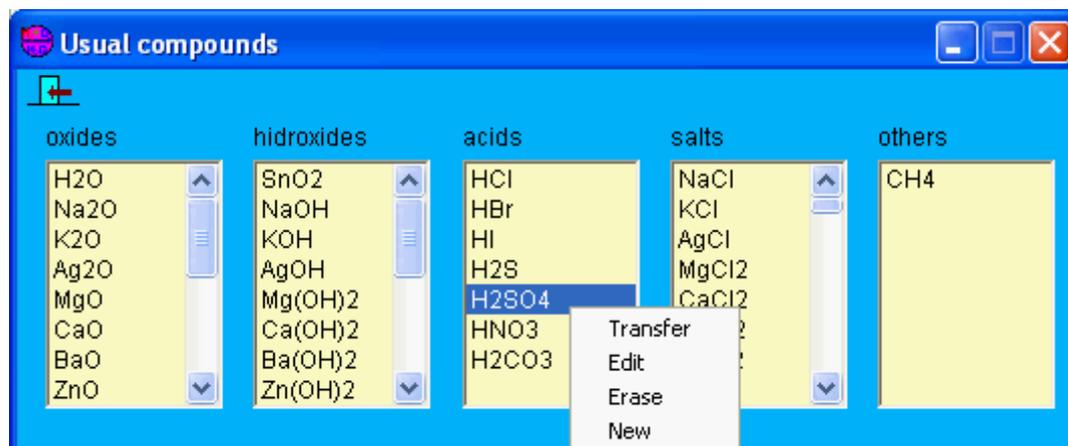
- **Add:** a new group or reaction by introducing it in its textbox (+Return)
- **Modify:** by selecting one from its list, editing it and Return
- **Erase:** by selecting it and clicking on the button 

Building /editing manually a chemical equation

Introducing the reactants and products in their textboxes, the chemical equation (not balanced) will be formed.



An option to introduce formulas without writing them is to invoke the window of compounds...



Here you have these options:

- **Transfer** selected formula to the main window
- **Edit** formula (and name)
- **Erase** compound
- **New**: incorporate new compounds



Balancing a reaction

Once obtained a reaction, we must balance its equation so that it reflects the proportion in mols of the implied compounds.

Reaction

$C_4H_{10} + O_2 \longrightarrow CO_2 + H_2O$

New Balance AutoBalance

• [Manual balancing](#)

• [Autobalancing](#)

Manual balancing: Click on

Then, the textboxes to introduce the coefficients of reactants and products are shown.

Reaction

C_4H_{10} + $O_2 \longrightarrow$ CO_2 + H_2O

New Accept AutoBalance

Clicking on the program will accept the balance if it is correct or it will show error messages if not .

Autobalancing: Clicking on the program will calculate the coefficients.

This option is not advisable from the point of view of learning, but it will be useful when you want to pass directly to the phase of calculations.

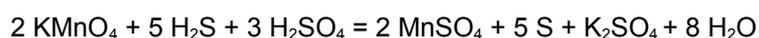
Anyway, you obtain the balanced equation:

Reaction

$2 C_4H_{10} + 13 O_2 \longrightarrow 8 CO_2 + 10 H_2O$

New Calculations AutoBalance

Note about autobalancing: the method is purely mathematical and, although rarely, in the Redox reactions can give a result mathematically correct but chemically false, that is: such that the number of electrons given by the reducer is different from the one captured by the oxidizer. An example: The reaction $KMnO_4 + H_2S + H_2SO_4 = MnSO_4 + S + K_2SO_4 + H_2O$, if balanced by the mathematic method gives $2 KMnO_4 + 2 H_2S + 2 H_2SO_4 = 2 MnSO_4 + S + K_2SO_4 + 4 H_2O$, that is compliant with the mass conservation, but balanced by the ion-electron method yields the chemically actual equation:



Calculations based on a (balanced) reaction:

Once balanced the equation, clicking on **Calculations** the textboxes for introduce data and present results will be shown.

You can introduce data of:

- One or more reactants (if more than one, the limiting reactant will be calculated).
- Or only one product (if more, they will be ignored).

The units of those (grams by default) can also be chosen here.

Clicking **OK** after the introduction, results are shown in the empty textboxes, and also a window that shows an outline of the “problem” formed:

```

REACTION: 2 C4H10 + 13 O2 = 8 CO2 + 10 H2O
=====
Data:
C4H10:  5 g . 1 mol/58.1g = 0.086059 mol / 2 -> 0.043029      <- Limiting R.
O2:     46 L at 1atm & 296°K = 1.895 mol / 13 -> 0.145784

Results:

REACTANT      reac. mols  - amount                excess ( = ini-reac.)
-----
O2            0.043029·13 = 0.55938· R·296K/1atm L/mol = 13.577L  -> 32.42 L

PRODUCT mols                amounts
-----
CO2           0.145784 × 8 = 0.344234  ·44g/mol = 15.15 g
H2O           0.145784 × 10 = 0.430293  ·18g/mol = 7.75 g
    
```

The problem can be saved in a file (in mode text). If the file already exists the problem will be added to it, and if not it will be created.