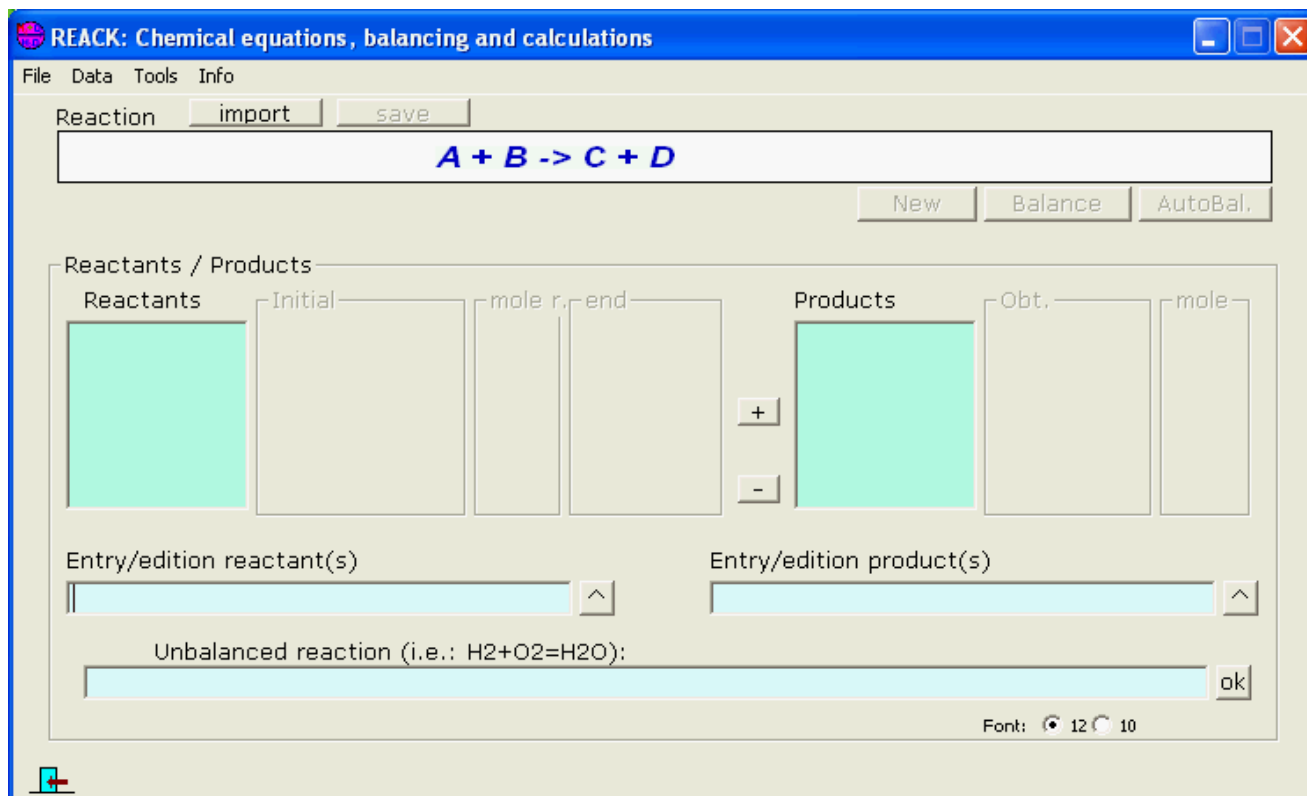


# REACK

## Balancing and calculations on chemical equations



- [Reactions: importing and editing](#)
- [Balancing a reaction](#)
- [Calculations on a chemical equation](#)
- [Problem](#)

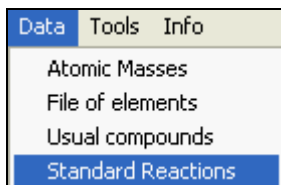
## Reactions: importing and editing

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 **Data** the option...



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

The 'Standard reactions' window contains the following elements and callouts:

- Group of reactions**: Points to the 'Type' dropdown menu.
- New group**: Points to the '+' button next to the 'Type' dropdown.
- Eliminate group**: Points to the 'x' button next to the 'Type' dropdown.
- Accept new**: Points to the 'ok' button next to the 'Type' dropdown.
- Search:**: A search input field with an 'ok' button.
- Reactions**: A list of reactions, with the first one highlighted in light blue.
- Selected reaction**: Points to the highlighted reaction in the list.
- New reaction**: Points to the '+' button next to the reaction list.
- Eliminate reaction**: Points to the 'x' button next to the reaction list.
- Accept new**: Points to the 'ok' button next to the reaction list.
- Description (optional)**: Points to the 'Descr.' dropdown menu.
- Transfer ->**: Points to the 'Transfer ->' button at the bottom right.

As you can see, here it's possible also modify and eliminate reactions and groups of them.

## Building / editing manually a chemical equation

Introducing the reactants and products in their textboxes, the (not balanced) chemical equation will be formed. Also you can enter the full reaction.

An option to introduce formulas without writing them is to invoke the window of **usual 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 moles of the implied compounds.

Reaction

$\text{C}_3\text{H}_8 + \text{O}_2 \longrightarrow \text{CO}_2 + \text{H}_2\text{O}$

propane combustion

- [Manual balancing](#)
- [Autobalancing](#)

**Manual balancing:** Click on

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

Reaction

$\text{C}_3\text{H}_8 +$    $\text{O}_2 \longrightarrow$    $\text{CO}_2 +$    $\text{H}_2\text{O}$

propane combustion

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.

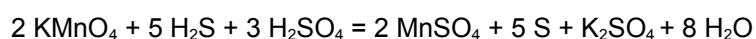
Anyway, you'll obtain the balanced equation:

Reaction

$\text{C}_3\text{H}_8 + 5 \text{O}_2 \longrightarrow 3 \text{CO}_2 + 4 \text{H}_2\text{O}$

propane combustion

**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  $\text{KMnO}_4 + \text{H}_2\text{S} + \text{H}_2\text{SO}_4 = \text{MnSO}_4 + \text{S} + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$ , if balanced by the mathematic method gives  $2 \text{KMnO}_4 + 2 \text{H}_2\text{S} + 2 \text{H}_2\text{SO}_4 = 2 \text{MnSO}_4 + \text{S} + \text{K}_2\text{SO}_4 + 4 \text{H}_2\text{O}$ , 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.

The screenshot shows the REACK software window titled "REACK: Chemical equations, balancing and calculations". The reaction is  $C_3H_8 + 5 O_2 \rightarrow 3 CO_2 + 4 H_2O$ , labeled "propane combustion". The "Calculations on the reaction" section is active. Reactants are listed as C3H8 (50 g) and O2 (200 L sc). Products are listed as CO2 and H2O. The atomic masses are given as A.M.: C = 12.01, H = 1.008, O = 16.00. The units are set to gram for C3H8 and L sc for O2. The pressure is 1.00 atm and temperature is 20.0 °C. The "Calc" button is highlighted.

Clicking on **Calc** after the introduction, results are shown in the empty textboxes:

The screenshot shows the same REACK software window after the calculation. The results are displayed in the "Calculations on the reaction" section. Reactants: C3H8 (50 g, 1.13 mole, 0.000g end), O2 (200 L sc, 5.67 mole, 73.0L sc end). Products: CO2 (150 g, 3.40 mole), H2O (81.7 g, 4.54 mole). The "Calc" button is highlighted.

**Problem:** Clicking on **Problem >** the problem will be shown:

The 'Problem' window displays the following content:

**Ennouncement**

C3H8 reacts with O2 to give: CO2 and H2O.  
 If are implied 50.0 g of C3H8 and 200 L cn of O2 calculate:  
 g of CO2 and g of H2O obtained .

**Resolution**

REACTION: C3H8 + 5 O2 = 3 CO2 + 4 H2O

=====  
 Data:  
 C3H8: 50.0 g x 1 mole/44.10g = 1.13 mole <- Limiting R.  
 O2: 200 L cn x 1 mole/22.4L = 8.93 mole / 5 -> 1.79

Results:

REACTANT	reac. moles	- amount	excess (= ini-reac.)
O2	1.13x5 = 5.67	5.67x 22.4L/mole = 127L cn	-> 73.0 L cn final

PRODUCT	moles	amounts
CO2	1.13x3 = 3.40	x44.01g/mole = 150 g
H2O	1.13x4 = 4.54	x18.02g/mole = 81.7 g

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

The 'File' menu in the 'Problem' window contains the following options:

- Save problem
- View file
- Exit

### Saving the reaction:

The entered reaction can be saved in the reactions database clicking on **save** :

The 'SAVE REACTION' dialog box includes the following fields and controls:

- Select TYPE or create +** (highlighted in orange) with an **ok** button.
- Type** field with a dropdown menu (currently showing 'random') and **+**, **x**, and **ok** buttons.
- Search:** field with an **ok** button and a **random** button.
- Reactions** dropdown menu (currently showing 'CH3CH2OH+O2=CO2+H2O').
- Sort** button.
- Optional: enter Description** (highlighted in orange) with an **Accept with ok** button.
- Descr.** dropdown menu.
- Transfer ->** button.

## Concentrations calculation

Option of **Tools** menu.

By selecting a compound from the list we can calculate, from the data of preparation of a solution their different expressions of concentration.

Also a form of concentration can be converted to others.

Tools	Info
Concentrations calculation	
Tools edition	
NotePad	
Windows calculator	

Compound: HCl MM: 36.46

Solution density: 1.06 g/ml

Preparation:

- g solute: 50
- solution ml: 500
- solvent g: 480

Concentration:

- Molarity: 2.74
- molality: 2.86
- g/l: 100
- Percent: 10.4

Buttons: OK, Calc

To convert a form of concentration to others: Enter it and click **Calc**

*Send any comment, suggestion or questions to:*

*[jog@scialt.com](mailto:jog@scialt.com)*

*More apps in the web: <http://www.scialt.com/en>*