

# CMOL

**Calculations on chemical formulas:** molar mass , conversions from grams to mols, molecules, volume of gas... Centesimal composition, empirical formula..

The screenshot shows the 'Calculations with mols' software interface. The main window displays the chemical formula  $C_{10}N_2H_{14}$  and its corresponding formula  $C_{10}N_2H_{14}$ . The molar mass calculation (MM) is shown as  $12.011 \times 10 + 14.007 \times 2 + 1.008 \times 14$ , resulting in a molar mass of 162.236 g/mol. The conversions section shows 3.56 grams converted to 0.02194 mols and 1.32e22 molecules. The composition section shows the centesimal composition: C 7.41, N 1.73, H 0.87, and a molar mass of 162. The interface includes buttons for 'Generate', 'Accept', 'Verify', 'Save composition', and 'Save empirical/mol. formula'.

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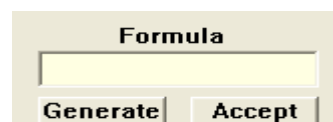
[Conversions](#)

[Centesimal composition](#)

[Empirical / molecular formula](#)

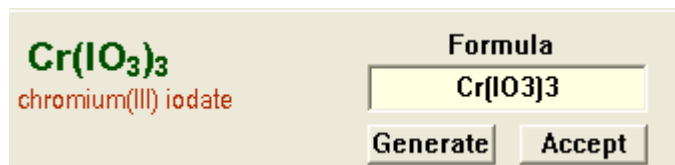
## Introducing/generating a formula

You can introduce the formula manually (without keeping in mind the format of subindexes, etc) whenever all their elements are in the database (which you can edit and enlarge)



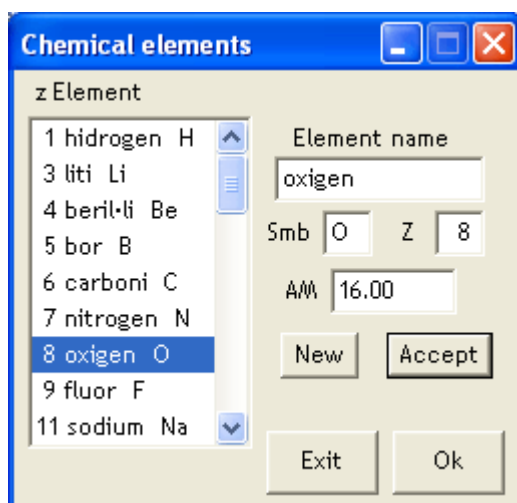
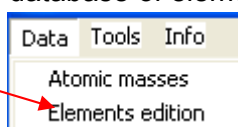
It can also be generated by the program and then the compound's name will also appear.

In both cases the formatted formula will appear to the left.



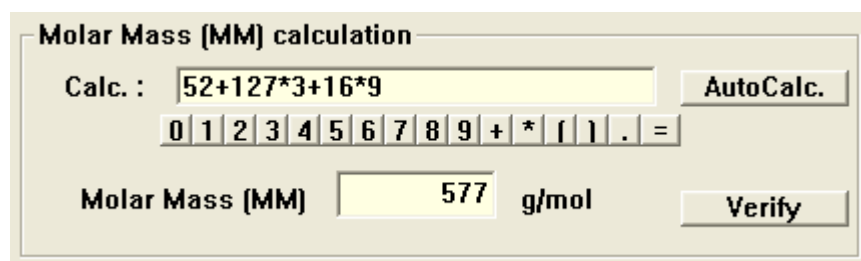
## Data

The calculations with the formulas use a database of elements that we can edit/enlarge with the option of the menu...



## Calculation of the molar mass

An option is to make the calculation and to check the result with the button **Verify**. Another is that the program calculates it by pressing the button **AutoCalc**.



## Conversions

You can select the type (grams, mols, " molecules "..) of the data that should be converted to the other types with the mouse

grams 42 1mol: MM g mols 0.07279 1mol: 6.02 · 10<sup>23</sup> "molecules" 4.38e22  
gas L. in C.N. 1mol: 22.4 L  
Generate Accept

If the substance is a gas (as CO<sub>2</sub>, CH<sub>4</sub>, etc...) you can activate the checkbox to also make calculations of volume in S.C.

Once introduced or generated the value of the original data, and depending of if you have also entered or not the conversions, if you press the button **Accept** the conversions will be calculated, and/or a list of erroneous entrances, if it proceeds, will be shown

grams 21 1mol: MM g mols 0.47717 1mol: 6.02 · 10<sup>23</sup> "molecules" 2.87e23  
gas L. in S.C. 10.69 1mol: 22.4 L  
Generate Accept

Erroneous or imprecise results  
mols 0.823  
molecules 4.25e23  
liters 18.7  
OK


(If you want see the correct values you must erase the wrong one and once click on Accept)

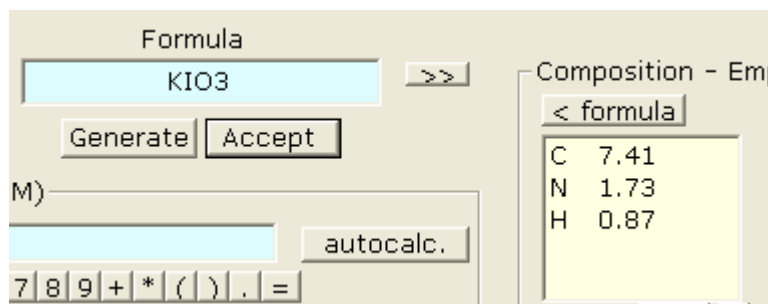
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### Note:

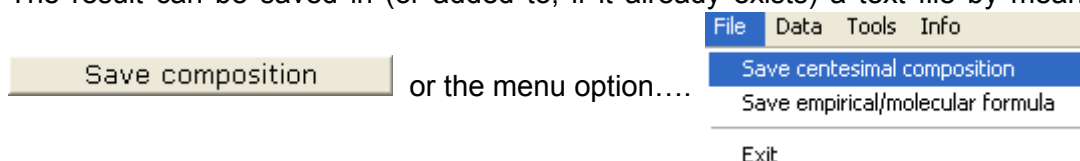
(\*): Ionic compounds (salts,...) aren't formed by actual molecules, but by groups of ions of opposite sign that are the smallest units of the compound.

## Centesimal composition

Once entered or generated a formula you can obtain its centesimal composition clicking on the button :



The result can be saved in (or added to, if it already exists) a text file by means the button

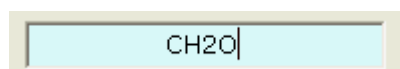


## Empirical / molecular formula

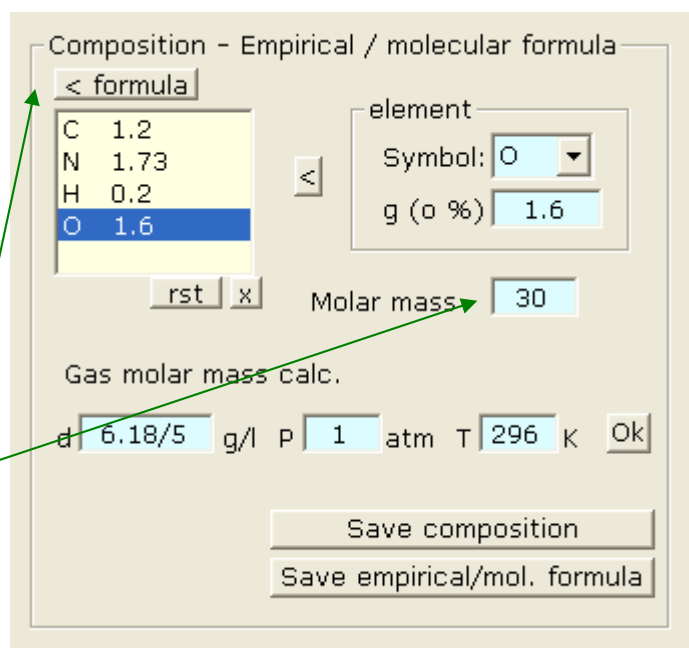
It can be obtained here:

Elements are entered or selected from the list, and also their amounts.

Once all elements are entered, clicking on the formula will be calculated and shown:



This will be the *empirical* (the simplest) or, if you have specified a molar mass, the *molecular* formula.



Molar mass of gaseous compounds can be calculated from their density (or from grams and volume expressed as a quotient) at certain pressure and temperature.

Also here the case can be saved in a text file...