

# CMOL

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

The screenshot displays the 'Calculations with mols' software window. The interface includes a menu bar (File, Data, Tools, Info) and a main workspace. At the top left, the chemical formula  $C_{10}N_2H_{14}$  is shown. Below it, a 'Formula' field contains 'C10N2H14' with 'Generate' and 'Accept' buttons. The 'Molar mass calculation (MM)' section features a calculator with the expression  $12.011*10+14.007*2+1.008*14$  and an 'autocalc.' button. The resulting 'Molar mass (MM)' is 162.236 g/mol, with a 'Verify' button. The 'Conversions' section has three radio buttons: 'grams' (selected), 'mols', and '"molecules"'. It shows conversions between 3.56 grams, 0.02194 moles, and  $1.32e22$  molecules, with conversion factors like '1mol: MM g' and '1mol: 6.02\*10<sup>23</sup>'. There are also options for 'gas' and 'L. in S.C.' with a '1mol: 22.4 L' factor. The 'Composition - Empirical / molecular formula' panel on the right shows a table of element percentages (C: 7.41, N: 1.73, H: 0.87) and a 'Molar mass' of 162. It includes buttons for 'Save composition' and 'Save empirical/mol. formula'.

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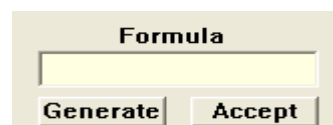
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## Introducing/generating a formula

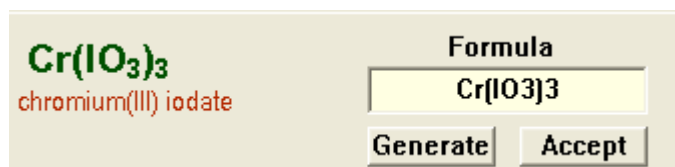
You can introduce the formula manually (without keeping in mind the format of subindexes, etc) whenever all their elements are in the database (which you can edit and enlarge)



A dialog box titled "Formula" with a text input field and two buttons: "Generate" and "Accept".

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

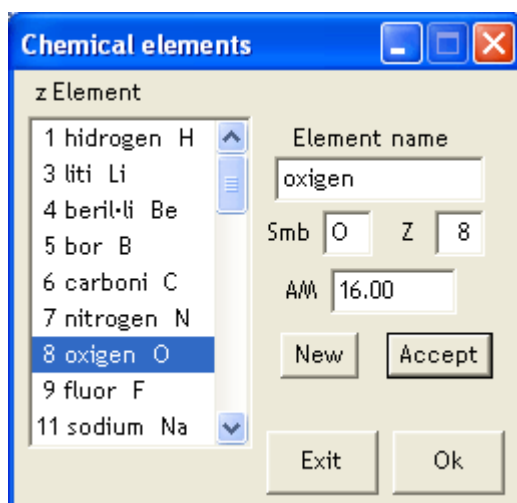
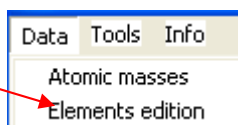
In both cases the formatted formula will appear to the left.



The result of formula generation for chromium(III) iodate. On the left, the chemical formula  $\text{Cr}(\text{IO}_3)_3$  is displayed in green, with the name "chromium(III) iodate" in red below it. On the right, a "Formula" dialog box shows the input "Cr(I03)3" and buttons "Generate" and "Accept".

## Data

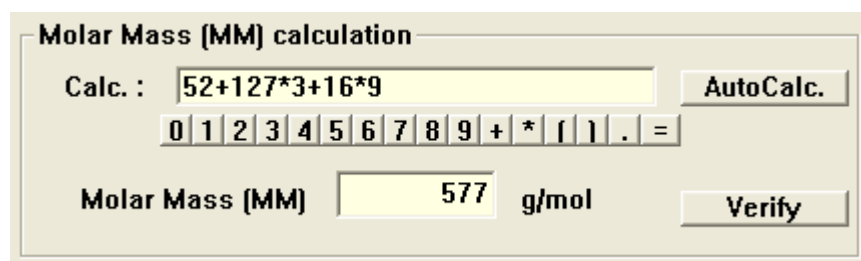
The calculations with the formulas use a database of elements that we can edit/enlarge with the option of the menu...



A dialog box titled "Chemical elements" with a list of elements on the left and input fields on the right. The list includes: 1 hydrogen H, 3 liti Li, 4 beril-li Be, 5 bor B, 6 carboni C, 7 nitrogen N, 8 oxigen O (highlighted), 9 fluor F, and 11 sodium Na. The right side has fields for "Element name" (containing "oxigen"), "Smb" (containing "O"), "Z" (containing "8"), and "AM" (containing "16.00"). There are buttons for "New", "Accept", "Exit", and "Ok".

## 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.**



A dialog box titled "Molar Mass (MM) calculation". It features a calculator interface with a display showing "52+127\*3+16\*9". Below the display is a row of buttons for digits 0-9, "+", "\*", "(", ")", ".", and "=". To the right of the calculator is an "AutoCalc." button. Below the calculator, the text "Molar Mass (MM)" is followed by a field showing "577" and "g/mol". To the right of this is a "Verify" button.

## Conversions

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

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.

Conversions

☒ grams ☐ mols ☐ "molecules"

42 0.07279 4.38e22

1mol: MM g 1mol: 6.02 · 10<sup>23</sup>

☐ gas ☐ L. in C.N.

1mol: 22.4 L

Generate Accept

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

Conversions

☒ grams ☐ mols ☐ "molecules"

21 0.47717 2.87e23

1mol: MM g 1mol: 6.02 · 10<sup>23</sup>

☒ gas ☐ L. in S.C.

1mol: 22.4 L

Generate Accept

Erroneous or imprecise results

mols 0.823  
molecules 4.25e23  
liters 18.7


OK

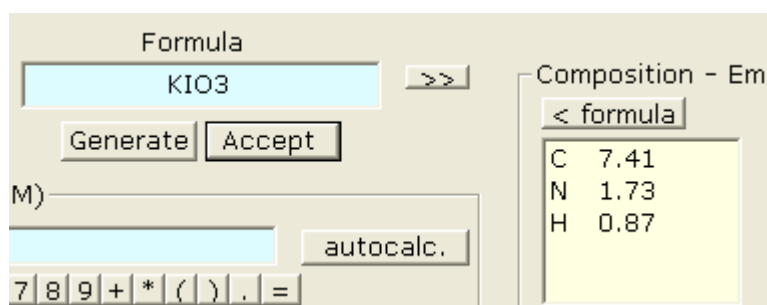
(If you want see the correct values you must erase the wrong one and once click on Accept)

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. Always we can say "formulas".

## Centesimal composition

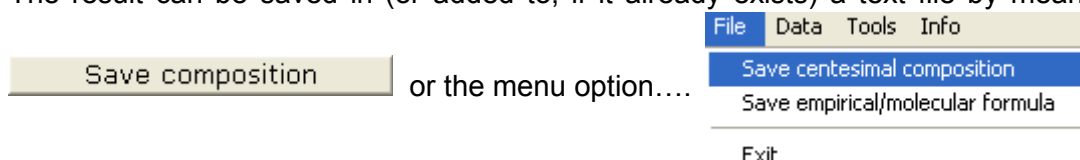
Once entered or generated a formula you can obtain its centesimal composition clicking on the button  :



The 'Formula' window displays the chemical formula KIO3 in the input field. Below it are 'Generate' and 'Accept' buttons. A numeric keypad is visible at the bottom. To the right, the 'Composition - Em' window shows the calculated centesimal composition:

< formula	
C	7.41
N	1.73
H	0.87

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



The 'Save composition' button is shown next to the 'File' menu. The menu options are:

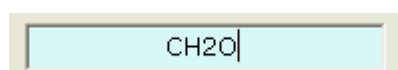
- File
- Data
- Tools
- Info
- Save centesimal composition
- Save empirical/molecular formula
- Exit

## Empirical / molecular formula

It can be obtained here:

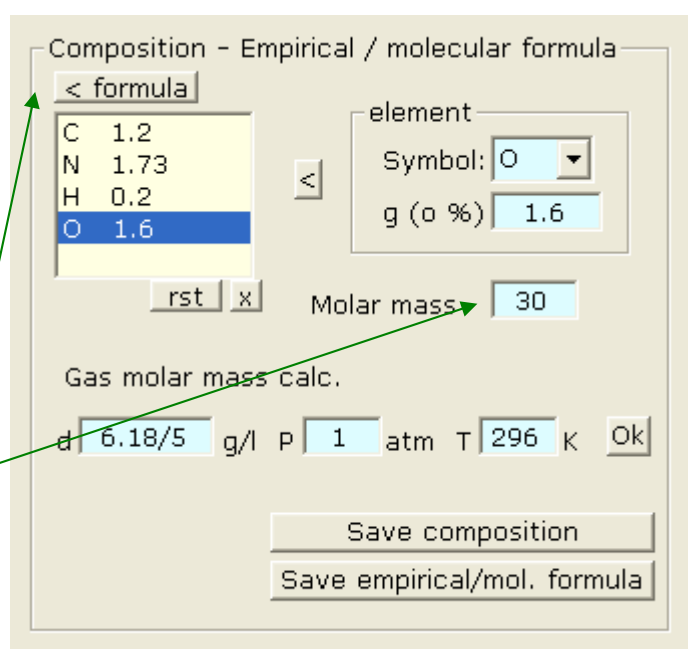
Elements are entered or selected from the list, and also their amounts.

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



The calculated formula CH2O is displayed in a text box.

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



The 'Composition - Empirical / molecular formula' window shows the input for calculating the formula. The 'element' list contains C (1.2), N (1.73), H (0.2), and O (1.6). The 'Molar mass' is set to 30. The 'Gas molar mass calc.' section includes density (d = 6.18/5 g/l), pressure (P = 1 atm), and temperature (T = 296 K). Buttons for 'Save composition' and 'Save empirical/mol. formula' are at the bottom.

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...