EniG. Chemistry Assistant version 2.0

We believe that you will find *Chemistry Assistant* to be easy to understand and use. Armed with a basic knowledge of how Windows programs work and some elementary understanding of the mathematic function, you should be able to easily take advantage of most of the features of the program.

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INTRODUCTION

Chemistry Assistant is an expression calculator for fast calculation of molecular weight of compounds by simple entry of chemical formula. The program translates the texts with chemical element symbols or without them into a mathematical expression and calculates them.

There is an intelligent routine which translates the symbols of elements written in small letters into correct chemical formula. The result of the translation will be entered into the entry field and calculated, or the programme will report error. The appearance of mathematical expression, which is the result of the translation, can be seen if the mouse pointer is held over the tasks field. The right mouse button has several often used anions and molecules.

The *Chemistry Assistant* contains a list with task history, storing all the recent inputs and results. All of the calculations can be saved and recalled again. The calculator also provides a list of common physical constants and performs various conversions between English and metric units.

System requirements: 32-bit PC with Windows 95, 98 or Windows NT operating system.

The author will appreciate to hear your comments, suggestions and bugs you may encounter.

For example, when calculate the relative molecular weight of a sodium(II) sulfate you type na2so4 and smart translator analyze and translate lower case typed chemical formula in correct form and calculates them.

```
na2so4 = Na2SO4
Na2SO4 = Na*2+S+O*4
Na*2+S+O*4 = 22.98977*2 + 32.066 + 15.9994*4
22.98977*2 + 32.066 + 15.9994*4 = 142.043
```

See also Entering expression Author

STATUS

EniG. Chemistry Assistant is FREEWARE software product.

You can use this program freely for private or business purposes, or distribute it to others, provided you do not gain any financial profits from it and provided you do not change the content of the files.

The program cannot be distributed for **commercial** purposes without prior consent from the author.

See also <u>Author</u> Install and uninstall

INSTALL AND UNINSTALL

Short web form

Distribution package

The distribution package (chemas20.zip) contains the following files:

Astronom.con	 astronomy constants
ChemAs.exe	- the calculation program itself
ChemAs.hlp	 help file for the program
Example.tsk	- sample calculations that can be loaded
File_id.diz	 short program description
Readme.txt	- program description

In order for the program to work, you need to have the files MSVBVM50.DLL and COMDLG32.OCX in the ../Windows/System directory. Those files are core libraries for programs written in Visual Basic 5.0.

Install short web form

Download *Chemistry Assistant*, and unpack (unzip) the files into a directory of your choice. Create a shortcut to the program in the Windows start menu, or on your desktop. There is no additional installation procedure.

You'll also need the files msvbvm50.dll and comdlg32.ocx, which are not in the package, but if you don't have them already, you can download them in a ZIP format from:

http://www.ktf-split.hr/~eni/toys/msvbvm50.zip

http://www.ktf-split.hr/~eni/toys/comdlg32.zip

and unzip in the ../Windows/System directory.

Uninstall short web form

Simply delete the files from disk.

Self-install package

Install self-install package

On the other hand, you can download a self-install copy of *Chemistry Assistant* with all the files needed. Unzip the files into a temporary directory and run setup program (setup.exe) from either the Windows Explorer or the Run option from the Start Menu.

Uninstall self-install package

Activate the Control Panel, double click Add/Remove Programs, and double click on the *Chemistry Assistant* list box entry.

Should you find any bugs, or in case you have any good ideas on improvements, please contact me by e-mail:

eni@ktf-split.hr

Enjoy!

The author shall not be responsible for any damages, direct or indirect, which may result from the use of this software.

See also Status Author

AUTHOR

Program:	EniG. <i>Chemistry Assistant</i>
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DISPLAY WINDOW

There are three main components of the display:

- <u>Status line</u>
- History area
- Input line



Status line

Status line is displayed across the top of the screen. Each item on the status line is one of the following:

- Number format
 - **AUTO** mode displays numbers exactly as you enter them and answers to 14 significant decimal places. **SCI** mode displays a number as a mantissa – with one digit to the left of the decimal point and the user-specified number of decimal places – and the exponent
 - FIX mode displays numbers rounded to a user specified number of decimal places (default is 2)
 - F5 key is the switch between different number formats
- Memory
 - The **MEM** sign appears when a number is stored in the memory
 - **F6** key stores the new result in the memory
 - F7 key recalls the value stored in the memory
- Angle measure

Controls the units in which angular measurements are interpreted: radians, degrees or grads.

- **RAD** The angle unit is set to radians
- DEG The angle unit is set to degrees
- **GRAD** The angle unit is set to grads
- F8 key is the switch between different units of angle measurement

History area

The history area shows input data and answers to last two calculations. All the expressions you create are stored on a scrolling list for later recall. Pres [?] button to display the task history and you can scroll through the history. The last expression is placed on the top of the history.

When the answer exceeds the normal display capacity, it is automatically shown in scientific notation with 14-digit mantissa and exponents of 10 up to 308.

Input line

There are four ways to insert an expression onto the input line:

- Type the expression directly onto the input line
- Use an expression from the history
- Load expression from the disk
- Use copy and paste an expression from another programs

To edit an existing expression, go on the input line, use the arrow keys to position the cursor where you want to insert the character, function or constant, and entering that.

When you have finished entering your expression, pres ENTER or click [=] button.

If the first character in the expression is **#** that is a command. With such expressions it is possible to change the number format or the angle measurement. For scientific mode with **3** decimal places enter **#sci3** in input line.

Examples

```
2+5-3.25 = 10.25
H2SO4 = 98.079
5! = 120
log1000 = 3
alog3 = 1000
x^2 + x -2 = 0 x1=1; x2=-2
```

See also

Entering expression Keyboard Menu Toolbar

KEYBOARD

Enter the number, chemical formulae, functions and operator just as you speak. To use your numeric keypad to enter numbers and operators, press **NUM LOCK**.

You enter a *positive number* by pressing the appropriate digit keys and, if necessary, the decimal point key [.].

Inverse functions can be inserted by clicking the left mouse button on a [INV] button then on the button associated with function.

Negative numbers are obtained by simple putting the character - before the number.

Enter the mantissa as the positive or negative number, and then click [EXP] button or just type E or e and type exponent as the positive or negative number.

Every *function* that is supported by *Chemistry Assistant* can be inserted by clicking on the button with function name or type its name on the physical keyboard. Some functions are not associated with the buttons, but every function can be called by typing its name.

If the first character in the expression is **#** that is a *command*. With such expressions it is possible to change the number format or the angle measurement. For scientific mode with **3** decimal places enter **#sci3** in input line.

To work with numbers stored in memory:

- Click MS to store a number. When you store a number in memory, an MEM appears in the Status line on the display.
- The number stored in the memory can be seen as a ToolTip text if the mouse pointer is held over the MEM sign.
- To recall a stored number, click [MR].
- If you store another number in memory, it replaces the number currently in memory.
- To clear the memory, click [INV] + [C].
- To add the displayed number to the number already in memory, click [M+]. Click [MR] to insert the new number.
- To subtract the displayed number to the number in memory, click [INV] + [M+]
- Clear memory
 - Store a zero in memory or click [INV] + [C] = [AC] clear memory and all statistical data

You must not enclose arguments in parentheses, except if arguments contain math operators.

Select the component you entered and then click the [(...)] button. *Chemistry Assistant* encloses the selected text in brackets or, if there is no selected text, encloses the whole expression in the input line.

Expand *Chemistry Assistant* can be used as a classic pocket scientific calculator. As a classic calculator *Chemistry Assistant* works only with the result of the last expression. If input line isn't empty, first the expression in the input line is calculated and then calculates the function from the Classic calculator.

See also Entering expression Basic calculations

MENU

This section describes the function of each menu item. Many menu items are shown with a keyboard shortcut. When such a shortcut is available, you may use the keyboard combination instead of choosing it in the menu.

<u>File menu</u> <u>Edit menu</u> <u>Insert menu</u> <u>View menu</u> <u>Help menu</u>

See also Display Window Keyboard Toolbar

FILE MENU

New CTRL+N

Clears display and all tasks stored in task history.

Open CTRL+O

Opens the tasks file and calculates them. The program reads and calculates line by line, ignoring all that appears after the equal sign (=).

Save As CTRL+S

All of the calculations can be saved and recalled again. The program saves complete task history with its results.

Print CTRL+P

Prints the task history with the belonging results.

Exit CTRL+Q Close Chemistry Assistant.

See also

Edit menu Insert menu View menu Help menu

EDIT MENU

Cut CTRL+X

Copies the selected text to the clipboard or, if nothing is selected, copies the whole expression in the input line, and then clears it from the input line.

Copy CTRL+C

Copies the selected text to the clipboard for pasting into other applications or, if nothing is selected, copies the last result from display to clipboard.

Paste CTRL+V

Copies the text from the clipboard and places it in the input line.

Delete SHIFT+DEL

Deletes the selected text or, if nothing is selected clear the input line.

Select All CTRL+A

Chemistry Assistant selects the whole expression in the input line.

Clear Display CTRL+Y

Clears display.

See also

<u>File menu</u> <u>Insert menu</u> <u>View menu</u> <u>Help menu</u>

INSERT MENU

The insert menu contains several often-used anions and molecules. This menu can be displayed as a popup menu after right clicking anywhere on the calculator keyboard.

List of anions and molecules in insert menu:

H2O	NO2	SO3
OH	NO3	SO4
CN	NH3	PO4
CH2	NH4	CrO4
CO3		Cr2O7

See also

<u>File menu</u> <u>Edit menu</u> <u>View menu</u> <u>Help menu</u>

VIEW MENU

Expand ChemAs

Use this option if you want to enlarge the dimension of the calculator. When the Expand ChemAs in View menu is unchecked the calculator goes back to its normal size.

Show Display only F12

F9

Use this option if you want to hide the calculator's keyboard and show Display only. **F12** key is the switch between different dimensions of the *Chemistry Assistant*.

Classic Calculator

Chemistry Assistant can be used as a classic pocket scientific calculator. As a classic calculator *Chemistry Assistant* works only with the result of the last calculation.

SI Units CTRL+U

Table with SI Units are based on the seven base units of the International System of Units: *m* (meter), *kg* (kilogram), *s* (second), *A* (ampere), *K* (kelvin), *cd* (candela), and *mol* (mole).

Physical Constants F11

Displays the table with over forty physical constants and you may insert them by double click of the chosen constant.

Custom Constants

Displays the table with prefixes SI units or, if loaded, displays your own custom constants.

New Custom Constants

Load new custom constants from the disk and change the table with prefix SI units.

Number format CTRL+F

Changes the displayed number formats and the unit of angle measurement.

Function separator

Use this option if you want to enable/disable the colon as function separator.

Always on top CTRL+T

Including this option *Chemistry Assistant* will be visible even when it is not active.

See also

<u>File menu</u> <u>Edit menu</u> <u>Insert menu</u> Help menu

HELP MENU

Help Topics

Chemistry Assistant also contains a detailed help file with syntax, usage, and examples for all of the supported functions. This help file opens on the contents page. Help is available at any time by pressing the F1 key.

"Tool Tips" are also available for buttons on the tool bar and keyboard by hovering over the button in question for more than 1 second.

Example

Loads and calculates the example task stored in the example.tsk file.

F1

Splash screen

Displays the introduce splash screen of the current version of Chemistry Assistant.

About

Displays a dialog in which some information about the current version of *Chemistry Assistant* is shown.

See also

<u>File menu</u> <u>Edit menu</u> <u>Insert menu</u> <u>View menu</u>

TOOLBAR

The toolbar allows quick access to some of the most useful features of *Chemistry Assistant*. The toolbar has 10 tool buttons, the function of which is provided in a ToolTip as the cursor is held over the button for a few seconds.



New

Clears complete task history.

Open	Opens the tasks file and calculates them.
Save	The program saves complete task history with its results.
Print	Prints the task history with the belonging results.
Cut	Copies the selected text to the clipboard or, if nothing is selected, copies the whole expression in the input line, and then clears it from the text box.
Сору	Copies the selected text or, if nothing is selected, the last result to the clipboard.
Paste	Copies text from the clipboard and places it in the input line.
Delete	Deletes the selected text or, if nothing is selected, clears the input line.
Number	format Changes the displayed number formats and the unit of angle measurement.
Expand	ChemAs Changes dimension of the calculator.

See also

<u>Display Window</u> <u>Keyboard</u> <u>Menu</u>

ENTERING EXPRESSION

Type your expression into the calculator just as you talk. Examples are available from Help menu (see <u>Example</u> tasks). Click on an example in task history to see its calculation.

There are four ways to insert an expression onto the input line:

- Enter the expression directly onto the input line
- Use an expression from the history
- Load expression from the disk
- Use copy and paste an expression from another programs

To edit an existing expression, go on the input line, use the mouse or the arrow keys to position the cursor where you want to insert the character, function or constant, and enter that.

When you finish entering your expression, pres **ENTER** or click [=] button.

Positive numbers

Enter a positive number by pressing the appropriate digit keys and, if necessary, the decimal point key [.].

Negative numbers

Negative numbers are obtained by simple putting the character - before the number.

Mantissa and exponents

Enter the mantissa as the positive or negative number, and then click [EXP] button or just type E or e and type exponent as the positive or negative number.

Functions

Every function that is supported by *Chemistry Assistant* can be inserted by clicking on button with function name or type its name on the physical keyboard. All supported functions are not assigned on buttons. To view the complete list of the function, go to <u>Math and trigonometry functions</u>. Function arguments do not have to be put in brackets, unless if it is defined as mathematical expressions.

Chemical formulae

The element symbols can be written in lowercase letters with the number of atoms after symbol, and the the program will translate them. If elements in chemical formula are properly capitalized smart case converter, leave them as you type. For indicating hydration you must use a + sign and leading number before formula is correct (CuSO4+5H2O).

Constants

Expand *Chemistry Assistant*, select constant tab and click the constant which you want to insert into expressions. You can load custom constants from the disk.

Power and root

Enter the number as the positive or negative number, and then click [^] button or just type ^ and type power as the positive or negative number.

Short key for power is **CTRL+**Number rising to power [^], (3**CTRL**2 = 3^2).

The root is obtained by raising the number to the reciprocal value of the root (1/x); for example, third root of 8 is $8^{(1/3)}=2$. Short key for root is **CTRL+SHIFT+Number** or **ALT+Number** (54**ALT**3 = cube root of a 54 or 54^(1/3))

Enter data from the history

You can also enter data onto the input line from history:

- 1. Press [?] button to display the task history.
- 2. Scroll the list until the data you want to copy to the input line is visible.
- 3. Click the left button of the mouse

Rules for typing expression

There are few rules for typing expression into the Chemical Assistant:

- Spaces are irrelevant, for example s in 45 is equal sin45
- Currency signs are ignored
- If you type a function without argument, the last result becomes a function argument
- If the first character in the expression is a math operator then the last result is put in before the math operator
- All types of parentheses are correct, for example 25.3/(K3[Fe(CN)6])
- It is not necessary to enclose the function argument into parentheses, except if arguments contain math operators, for example log100 or sin(pi/2)
- For indicating hydration you must use a + sign, for example CuSO4+5H2O
- It is correct to type the leading number before formula: 3CO2 is equal 3*(CO2)
- It is correct to type the leading number before parenthesis or function: 3(5.6-2.3) is equal **3*(5.6)-2.3**) or **4**log125 is equal **4*log125**
- Use standard calculator notation for scientific notation, for example 1e-5 is 0.00001; 1e+3 or 1e3 is 1000

Smart case conversion

The element symbols can be written in lowercase letters, and the intelligent routine in the program will try to translate them and will show the result of translation - or it will report an error. If elements in a chemical formula are properly capitalized, the smart case converter leaves them as you have typed.

The appearance of mathematical expression, which is the result of the translation, can be seen if the mouse pointer is held over the tasks field.

Implied multiplication

When you enter an expression, you press [x] button or * key to specify multiplication. For certain expressions, Chemical Assistant assumes that multiplication is intended and you do not need to specify it. This is the case in the following situations:

- A number followed by a chemical element, for example 2H2O is equal 2*(H2O)
- A number followed by an opening parenthesis, for example 2(8-5) is equal 2*(8-5)
- A number followed by a prefix function, for example 2sin45 is equal 2*sin(45)

See also

Basic calculations Molecular weight calculations Math and trigonometry functions Quadratic equation Statistical analyses Scientific constants

BASIC CALCULATIONS

Operations with the same precedence are performed from left to right, with operations enclosed in parentheses performed first. If parentheses are nested, the operations enclosed in the innermost set of parentheses are performed first.

Arithmetic operators

To perform basic mathematical operations such as addition, subtraction, or multiplication, use the following arithmetic operators:

Operator	Sign	Meaning	Example
+	plus sign	Addition	8+3
_	minus sign	Subtraction / Minus sign	5–2
*	asterisk	Multiplication	3*3
/	forward slash	Division	3/3
%	percent sign	Percent	20%750
^	caret	Power	3^2

Negative numbers are obtained by putting the character – before the number, $(2^*-3 = -6.)$

Enter the number as the positive or negative number, and then click [^] button or just type $^$ and type power as the positive or negative number. Also, you can type a double multiplication ** which will be replace by rising to power ^, (2**3 = 2^3 = 8).

Shortcut key for power is CTRL+Number rising to power, (3CTRL2 is equal 3^2).

The root is obtained by raising the number to the reciprocal value of the root (1/x); for example, third root of 8 is $8^{(1/3)}=2$.

Shortcut key for root is CTRL+SHIFT+Number or ALT+Number (54ALT3 is equal cube root of a 54 or 54^(1/3))

The [(...)] button will put the selected text or, if nothing is selected, the whole expression into parentheses in the entry field.

All of the calculations can be saved and recalled again, or a new task can be read from disk. The program reads and calculates line by line, ignoring all that appears after the equal sign =.

Examples

```
2+5-3.25 = 10.25
8+7+(42-16)*3 = 90
8+7+[(42-16)-7]*3 = 72
5*-7 = -35
7e-6/3e-9 = 2333.3333333333
5%40 = 2
8**3 = 8^3 = 512
2^-3 = 0.125
```

See also

Entering expression Molecular weight calculations Math and trigonometry functions Quadratic equation Statistical analyses Scientific constants

MOLECULAR WEIGHT CALCULATIONS

Chemistry Assistant translates the chemical formula into mathematical text, and replaces the element symbols with their atomic weight. The appearance of mathematical expression, which is the result of the translation, can be seen if the mouse pointer is held over the tasks field.

The element symbols can be written in lowercase letters, and the intelligent routine in the program will try to translate them and will show the result of translation - or it will report an error.

The right mouse button has several often-used anions and molecules.

- for indicating hydration using [+] sign CuSO4+5H2O
- leading number is correctly typed before formula: 3CO2
- it is also possible to use all types parentheses to define the chemical formula

The relative molecular weight of the substance will be defined as the sum of relative atomic weights of the elements, multiplied by the number of atoms in the formula of this substance.

Any atom in periodic system can be used in the chemical formula. The symbol of the atom is a capital letter if it consists of only one character, such as S for Sulfur or N for Nitrogen. If the symbol consists of two characters then only the first one is a capital letter, such as S for Silicon or Na for Sodium.

For example, when manual calculating the relative molecular weight of lead(II) nitrate, you must type the correct chemical formula

Pb(NO3)2

Make a list of each element and the number of atoms of each element present in the substance:

Pb×1 N×1×2 O×3×2

Go to periodic table and determine the relative atomic weights of each element, and multiply by the number of atoms in the formula:

Pb 207.2×1 = 207.2 N 14.00674×2 = 28.01348 O 15.9994×6 = 95.9964

Sum of weights of the each elements give relative molecular weight of the lead(II) nitrate. Pb (NO3)2 = 207.2 + 28.01348 + 95.9964 = 331.2

Since the relative atomic weight of lead given above only has 1 decimal place, accuracy cannot be determined beyond that point.

When calculating the relative molecular weight of a copper(II) sulfate pentahydrate, type

cuso4+5h2o

And the smart converter will translate this text in the correct chemical formula CuSO4+5H2O

If the chemical formula contains a mathematical operator (such as +, *, /, ...), smart converter will automatic add the parentheses in the expression

```
(CuSO4) +5* (H2O)
The next step is the change of chemical symbols with the molecular weight for each element
(63.546+32.066+15.9994*4) +5* (1.00794*2+15.9994)
The least step is calculate this expected methometical supression
```

```
The last step is calculate this created mathematical expression
```

(63.546+32.066+15.9994*4)+5*(1.00794*2+15.9994) = 249.686and display task and results

(CuSO4)+5*(H2O)

249.686

Examples

```
h2so4 = H2SO4
H2SO4 = H*2+S+O*4 = 1.00794*2+32.066+15.9994*4
H*2+S+O*4 = 1.00794*2+32.066+15.9994*4
1.00794*2+32.066+15.9994*4 = 98,079
```

See also

Entering expression Basic calculations Math and trigonometry functions Quadratic equation Statistical analyses Scientific constants

MATH AND TRIGONOMETRY FUNCTIONS

Every function that is supported by *Chemistry Assistant* can be inserted by clicking on button with function name or type its name on the physical keyboard. All supported functions are not assigned on buttons.

In trigonometric calculations, angles are interpreted as radians (default), degrees or grads, depending on Mode setting (DEG, RAD or GRAD mode).

1	Returns the factorial of a number
abs	Returns the absolute value of a number
acos	Returns the arccosine of a number
acot	Returns the arc cotangent of a number
<u>aln</u>	Returns natural antilogarithm
alog	Returns common antilogarithm
ans	Returns the last result
<u>asin</u>	Returns the arcsine of a number
<u>atan</u>	Returns the arctangent of a number
COS	Returns the cosine of a number
<u>cot</u>	Returns the cotangent of the given angle.
<u>dat</u>	Adding data for statistical analyses
<u>int</u>	Rounds a number down to the nearest integer
<u>ln</u>	Returns the natural logarithm of a number
log	Returns the base-10 logarithm of a number
mem	Recalls the value stored in the memory
pi	Returns the value of Pi
<u>ppm</u>	Returns the parts per million of a number
<u>ran</u>	Returns a random number
<u>sgn</u>	Returns an integer indicating the sign of a number.
<u>sin</u>	Returns the sine of the given angle
<u>sqrt</u>	Returns a positive square root
<u>tan</u>	Returns the tangent of a number

See also

Entering expression Basic calculations Molecular weight calculations Quadratic equation Statistical analyses Scientific constants

Į.

Returns the factorial of a number. The factorial of a number is equal to 1*2*3*...* number.

Syntax

x!

x is the nonnegative number you want the factorial of, and must be lower or equal to 170. If number is not an integer, it is truncated.

Examples

```
1! = 1

1.9! = 1! = 1

0! = 1

5! = 1*2*3*4*5 = 120

-1! = Error

171! = Result is too large!
```

See also

Math and trigonometry functions

abs

Returns the absolute value of a number. The absolute value of a number is the number without its sign.

Syntax

abs(x) abs x :abs x

x is the real number of which you want the absolute value.

Examples

```
abs2 = 2
abs-8 = 8
sqrt(abs(-25)) = 5
sqrtabs-25 = 5
```

See also

Math and trigonometry functions

acos

Returns the arccosine of a number. The arccosine is the angle whose cosine is number. The returned angle is given in radians in the range 0 (zero) to Pi.

Syntax

arccos(x) arccos x :arccos x acos(x) acos x :acos x

x is the cosine of the angle you want and must be from -1 to 1.

Examples

pi

```
If the angle unit is set to radians
    a\cos(0.5) = 1.0472 radians
```

if the angle unit is set to degrees

 $a\cos(0.5) = 120$ degrees

if the angle unit is set to grads acos(0.5) = 66.7 grads

See also Math and trigonometry functions <u>acot</u> <u>asin</u> <u>atan</u> <u>cos</u> cot <u>sin</u> <u>tan</u>

acot

Returns the arc cotangent of a number. The arc cotangent is the angle whose cotangent is number. The returned angle is given in radians in the range -pi/2 to pi/2.

Syntax

arccot(x) arccot x :arccot x acot(x) acot x :acot x actg(x) actg x :actg x

x is the cotangent of the angle you want.

Examples

See also

Math and trigonometry functions acos asin atan cos cot sin tan

pi

aln

Returns e raised to the power of number. The constant **e** equals 2.71828182845904, the base of the natural logarithm. **aln** is the inverse of **In**, the natural logarithm of number. To calculate powers of other bases, use the exponentiation operator ($^{\circ}$).

Syntax

aln(x) aln x :aln x exp(x) exp x :exp x

x is the exponent applied to the base **e**.

Examples

```
aln(1) equals 2.718282 (the approximate value of e) aln(2) = e^2 or 7.389056 aln(ln(3)) = 3
```

See also

<u>Math and trigonometry functions</u> <u>alog</u> <u>log</u> <u>In</u>

alog

Returns 10 raised to the power of number. **alog** is the inverse of **log**, the common logarithm of number. To calculate powers of other bases, use the exponentiation operator (^).

Syntax

alog(x) alog x :alog x

x is the exponent applied to the base **e**.

Examples

```
alog(1) equals 10
alog(2) = 100
alog(log(3)) = 3
alog(1E-5) = -5
```

See also

<u>Math and trigonometry functions</u> <u>aln</u> log ln

ans

ans is the equivalent to the result of the last expression. You can compose a task file in which each line contains the result computed in the line before.

Syntax

ans :ans

Examples

```
5*2 = 10
log(ans^2) = log(10^2) = 2
log(ans^2) = log(2^2) = 0.602
log(10^ans) = log(10^20.602) = 0.602
5*2 = 10
ans/2+ans/3 = 10/2+10/3 = 8.333
```

See also

Math and trigonometry functions

asin

Returns the arcsine of a number. The arcsine is the angle whose sine is number. The returned angle is given in radians in the range -pi/2 to pi/2.

Syntax

arcsin(x) arcsin x :arcsin x asin(x) asin x :asin x

x is the sine of the angle you want and must be from -1 to 1.

Examples

pi

```
If the angle unit is set to radians
asin(0.5) = 0.5236 radians
```

If the angle unit is set to degrees

asin(0.5) = 30 degrees

See also Math and trigonometry functions <u>acos</u> <u>acot</u> <u>atan</u> <u>cos</u> cot <u>sin</u> <u>tan</u>

atan

Returns the arctangent of a number. The arctangent is the angle whose tangent is number. The returned angle is given in radians in the range -pi/2 to pi/2.

Syntax

arctan(x) arctan x :arctan x atan(x) atan x :atan x atg(x) atg x :atg x

x is the tangent of the angle you want.

Examples

```
If the angle unit is set to radians
    atan(1) = 0.7854 radians
```

If the angle unit is set to degrees atan(1) = 45 degrees

If the angle unit is set to grads atan(1) = 50 grads

See also

Math and trigonometry functions <u>acos</u> <u>acot</u> <u>asin</u> COS <u>cot</u> <u>sin</u> <u>tan</u>

pi

COS

Returns the cosine of the given angle.

Syntax

cos(x) cos x :cos x

x is the angle in radians for which you want the cosine.

Examples

If the angle unit is set to radians $\cos(1) = 0.540$

If the angle unit is set to degrees $\cos(45) = 0.707$

If the angle unit is set to grads $\cos (45) = 0.760$

See also

Math and trigonometry functions acos acot asin atan cot sin tan pi

cot

Returns the cotangent of the given angle.

Syntax

cot(x) cot x :cot x ctg(x) ctg x :ctg x

x is the angle in radians for which you want the cotangent.

Examples

```
If the angle unit is set to radians
cot(1) = 0.6421
```

If the angle unit is set to degrees $\cot(45) = 1$

If the angle unit is set to grads cot(45) = 1.1708

See also <u>Math and trigonometry functions</u> <u>acos</u> <u>acot</u> <u>asin</u> <u>atan</u> <u>cos</u> <u>sin</u> <u>tan</u> <u>pi</u>

int

Rounds a number down to the nearest integer.

Syntax

int(x) int x :int x

x is the real number you want to round down to an integer.

Examples

int(8.9) = 8
int(8.1) = 8
int(-8.9) = -9
int(-8.1) = -9

See also

Math and trigonometry functions

In

Returns the natural logarithm of a number. Natural logarithms are based on the constant **e** (2.71828182845904). **In** is the inverse of the **exp** function.

Syntax

In(x) In x :In x

x is the positive real number for which you want the natural logarithm.

Examples

ln(100) = 4.6052 ln(2.7182818) = 1 ln(exp(7)) = 7

See also

<u>Math and trigonometry functions</u> aln alog log

log

Returns the common (base-10) logarithm of a number.

Syntax

log(x) log x :log x

x is the positive real number for which you want the base-10 logarithm.

Examples

```
log(1000) = 3
log(426) = 2.6294
log(1E-5) = -5
log(10^{5}) = 5
```

See also

Math and trigonometry functions aln alog In

mem

Recalls the value stored in the memory.

Syntax

mem :mem

If you want store another number (last result) in memory, you must enter the command:

#mem

If you want add or subtract result to number into memory, you must enter the command:

#mem+ #mem-

Examples

5*20 = 100 #mem = 100 log mem = 2 #mem+ = 102 mem*3 = 306 #mem- = -204

See also

Math and trigonometry functions

рі

Returns the value of mathematical constant pi, 3.1415926535898, accurate to 14 digits

Syntax

pi :pi

Examples

pi/2 = 1.57079 sin(pi/2) = 1

If the radius of a circle is Radius, the following formula calculates the area of the circle:

Radius^2 * pi = Area

See also

Math and trigonometry functions Scientific constants acos acot asin atan cos cot sin

<u>tan</u>

ppm

Returns the parts per million of a number

Syntax

ppm(x) ppm x :ppm x

The required number argument (x) can be any valid numeric expression.

Examples

ppm(450) = 0.00045 ppm(1E6) = 1

See also

Math and trigonometry functions

ran

Returns an evenly distributed random number greater than or equal to 0 and less than x.

Syntax

ran(x) ran x :ran x

The required number argument (x) can be any valid numeric expression.

Examples

```
If you want random number greater than or equal to 0 and less than 2 ran(2) = 1,44377934932709
```

If you want integer random number greater than or equal to 0 and less than 100 ran(int(100)) = 45

See also Math and trigonometry functions

sin

Returns the sine of the given angle.

Syntax

sin(x) sin x :sin x

x is the angle in radians for which you want the sine.

Examples

If the angle unit is set to radians sin(1) = 0,84147

if the angle unit is set to degrees
 sin(45) = 0.707

if the angle unit is set to grads sin(45) = 0.649

See also

Math and trigonometry functions acos acot asin atan cos cot tan pi

sgn

Returns an integer indicating the sign of a number.

Syntax

sgn(x) sgn x :sgn x

The required number argument (x) can be any valid numeric expression.

Return Values

lf number is	Sgn returns
Greater than zero	1
Equal to zero	0
Less than zero	-1

Examples

```
sgn(9.37) = 1

sgn(-25) = -1

sgn(0) = 0
```

See also

Math and trigonometry functions

sqrt

Returns a positive square root.

Syntax

sqr(x) sqr x :sqr x sqrt(x) sqrt x :sqrt x

Number is the number for which you want the square root. If number is negative, sqrt returns the error value.

Shortcut key for square root is CTRL+SHIFT+2 or ALT+2 (25ALT2 is equal square root of a 25 or 25^(1/2) = 5)

Generally, shortcut key for root is CTRL+SHIFT+Number or ALT+Number (54ALT3 is equal cube root of a 54 or 54^(1/3))

Examples

```
sqrt(9) = 3
sqrt(-25) = Error - negative number!
sqr abs-25 = 5
```

See also

Math and trigonometry functions

tan

Returns the tangent of the given angle.

Syntax

tan(x) tan x :tan x tg(x) tg x :tg x

The required number argument (x) can be any valid numeric expression.

Examples

```
If the angle unit is set to radians

tan(1) = 1,5574

if the angle unit is set to degrees

tan(45) = 1

if the angle unit is set to grads

tan(45) = 0,8541
```

See also <u>Math and trigonometry functions</u> <u>acos</u> <u>acot</u> <u>asin</u> <u>atan</u> <u>cos</u> <u>cot</u> <u>sin</u> <u>pi</u>

QUADRATIC EQUATION

Use function $[x^2+x=0]$ for solving the quadratic equation in form: $ax^2+bx+c=0$:

Displayed results can be:

Example	Result	Description
x^2+x-2=0	x1 = 1; x2 = -2	Two different real results
x^2+2x+1=0	x1 = x2 =1	Only one result (double)
$x^2 + 4x + 8 = 0$	x1 = x2=Complex number	Non-real results

Examples

```
4E-3x^2+3E-2x-2E-2=0
4x^2-3x-2=0
x^2+x-2=0
x^2-4=0
```

See also

Entering expression Basic calculations Molecular weight calculations Math and trigonometry functions Statistical analyses Scientific constants

STATISTICAL ANALYSES

When you analyze data statistically the data you create is stored in the [sum] variable. Use the [sum] function to calculate values such as the mean value, the sample and population standard deviation.

Syntax

In sum function only + or - signs may be used for separating the data!

```
sum(x1 + x2 + x3+ ...)
sum x1 + x2 + x3+ ...
:sum x1 + x2 + x3+ ...
```

Adding data for statistical analyses.

dat(x) dat x :dat x

Type sum without arguments to view the statistical analysis your data.

sum :sum

Clear the data from previous calculations through type a

sum 0

[INV] + [C] = [AC] - clear memory and sum variable

Returned value

or

After the statistical analysis a display will appear with the following results:

sum (x1, x2,)	Sum of all x values.
n	Number of data
S	Sample standard deviation
Mean	Mean of all x values.

The sample standard deviation is defined as

$$s = \sqrt{\frac{\sum x^2 - \frac{(\sum x)^2}{n}}{n-1}}$$

The population standard deviation is defined as

$$c\tau = \sqrt{\frac{\sum x^2 - \frac{\left(\sum x\right)^2}{n}}{n}}$$

And the arithmetical mean is defined as

$$\overline{x} = \frac{\sum x}{n}$$

Examples

sum(4.3+4.8+4.7+4.7) = 18.5; n=4; s=4.625; Mean=0.221735578260835dat(4.5) = 4.5 sum = sum(4.3+4.8+4.7+4.7+4.5) = 23; n = 5; s = 4.6; Mean = 0.2

See also

Entering expression Basic calculations Molecular weight calculations Math and trigonometry functions Quadratic equation Scientific constants

SCIENTIFIC CONSTANTS

Chemistry Assistant can be used as common scientific calculator, but it also includes a molecular weight calculator and the tables with various physical and chemical constants.

Clicking the Constants button located on the top expand of *Chemistry Assistant* or through the *View menu* item, you get access physical constants table. There are over forty physical constants in the table and you may insert a constant by double click the chosen constant.

The *Chemistry Assistants* table with SI Units are based on the 7 base units of the International System of Units: *m* (meter), *kg* (kilogram), *s* (second), *A* (ampere), *K* (kelvin), *cd* (candela), and *mol* (mole). You select a unit by pressing [SI Units] button, choosing the appropriate category from the Units list (length, area, volume, etc.) and finally selecting the unit. You do this when converting one unit to another.

See also
<u>Entering expression</u>
<u>Basic calculations</u>
<u>Molecular weight calculations</u>
<u>Math and trigonometry functions</u>
<u>Quadratic equation</u>
<u>Statistical analyses</u>
<u>pi</u>

EXAMPLE TASKS

Chemistry Assistant reads and calculates line by line, ignoring all that appears after the equal sign [=]. The lines which started with **#** are command lines. With these lines it is possible to change the number format or the angle measurement.

Here are the sample tasks divided in several categories:

Basic calculations Calculate function Calculate chemical formula Combine expressions

```
= Basic calculations
3+3 = 6
5+7+10+2 = 5+7+10+2 = 24
12+(20-8)*3+7 = 55
(8+3 = Missing right bracket ')' !
12+2+8)*3+7 = Missing left bracket '(' !
2+2-9 = -5
.5*, 6 = 0.5*0.6 = 0.3
2.5+2.12+-9*.8 = 2.5+2.12-9 = -2.58
27/3 = 9
3*5*7 = 105
9.12E-31*5 = 4.56E-30
9.12E+3+5.1e-1 = 9.12E3+5.1E-1 = 9120.51
5.48E-7/5.972E24 = 9.17615539182853E-32
2**3 = 2^3 = 8
2^{3}/0 = Cannot divide by zero!
8.12E-5/2 = 0.0000406
8.12E5/2 = 406000
4+5-*-1 = Type mismatch
4++5--7 = 4+5-1*-7 = 16
= Calculate functions
:sin1.5 = 0.997494986604054
:asin = :asin(Last answer) = :asin0.997494986604054 = 1.5
\cos 2 = :\cos 2 = -0.416146836547142
:tan5 = -3.38051500624659
:cot2 = -0.457657554360286
:log1000 = 3
alog3 = :alog3 = 1000
5! = 120
:ran100 = 33.9901149272919
:int(:ran100) = 45
:ln123 = 4.81218435537242
:\log 543E-8 = -5.26520017041115
:\log 5.43E-8 = -7.26520017041115
:log(5-8) = Logarithm of a negative number!
logabs(5-8) = :log:abs(5-8) = 0.477121254719662
15\%60 = 9
15ppm600 = 15*:ppm600 = 0.009
x^2 + x = 0 = x1 = 0; x2 = -1
x^2 + x - 7 = 0 = x1 = 2.19258240356725; x2 = -3.19258240356725
:sum(5.5+5.6+5.56+5.68+5.64) = 27.98; n = 5; s = 5.596; Mean = 6.98569967862918E-02
:dat5.82 = :sum(5.5+5.6+5.56+5.68+5.64+5.82)
dat(1,8*3) = : sum (5.5+5.6+5.56+5.68+5.64+5.82+5.4)
:Sum = :sum(5.5+5.6+5.56+5.68+5.64+5.82+5.4) = 39.2; n = 7; s = 0.134164078649987; Mean
= 5.6
```

= Calculate chemical formula

```
H2SO4 = H*2+S+O*4 = 1.00794*2+32.066+15.9994*4 = 98.079
h2o = H2O = 18.0153
cu(no3)2 = Cu(NO3)2 = 63.546+(14.00674+15.9994*3)*2 = 187.556
ch3ch2cooh = CH3CH2COOH = 74.0785
clch2ch2cohcl = ClCH2CH2COHCl = 127.9766
nabio3 = NaBiO3 = 279.9684
hno3 = HNO3 = 63.0129
naso4 = NaSO4 = 119.053
CoAsO4 = 197.8524
wrco3 = WRCO3 = R isn't chemical symbol!
cuso4+5h20 = (CuSO4)+5*(H2O) = 260.4036
```

= Command and combine expressions

73.9/nano3 = 73.9/(NaNO3) = 0.869465876170411 pb(no3)2+2h2o = (Pb(NO3)2)+2*(H2O) = 367.24044 al(no3)2+2h2o = (Al(NO3)3)+9*(H2O) = 375.133878

```
#fix3 = numbers rounded to three decimal places
(Cr(NO3)3)+9*(H2O) = 400.148
```

```
(Fe(NO3)3)+9*(H2O) = 403.140
(Fe(NO3)3)+9*(H2O) = 403.997
#sci1 = scientific mode with one decimal place
(Ni(NO3)2)+6*(H2O) = 2.9 E+02
(Mn(NO3)2)+6*(H2O) = 2.9 E+02
#auto = return to automatic mode
(Ni(NO3)2)+6*(H2O) = 290.79496
(Mn(NO3)2)+6*(H2O) = 287.039609
```

```
sin2=0.90929742682568
#fix3
sin2=0.909
#fix3 deg
sin2=0.035
#sci5grad
```

sin2=3.14108 E-02

```
#auto rad
Ca(NO3)2 = 164.088
Sr(NO3)2 = 211.63
104.4/(mn(no3)2+6h2o) = 104.4/(Mn(NO3)2+6*(H2O)) = 0.363712870024151
naf = NaF = 41.988173
intnaf = :int(NaF) = 41
lognaf = :log(NaF) = 1.6231269799864
```

See also

Entering expression Basic calculations Molecular weight calculations Math and trigonometry functions Quadratic equation Statistical analyses

NUMBER FORMAT

You can use number formats to change the appearance of numbers without changing the number behind the appearance. The number display defaults to *Auto mode*. You can change the display by choosing, in *View* menu, *Number Format*, or click on the **.00** icon.

The lines which started with # are command lines. With these lines it is possible to change the number format or the angle measurement. For scientific mode with 5 decimal places enter **#sci5** in input line.

Only in Fix mode Chemistry Assistant will make differences of the period and comas.

Auto mode #auto

If you activate this option *Chemistry Assistant* will automatically determine the number display of the result. The range of real numbers is from -1.7E+308 to 1.7E+308 with 14 decimal places.

Scientific mode #scix

Scientific mode displays a number as a mantissa, with one digit to the left of the decimal point and a user-specified number of decimal places, and an exponent. For example, 1234 appears as 1.23400 E+03 in scientific mode with 5 decimal places.

Fix mode #fixx

Fix mode displays the numbers rounded to a user-specified number of decimal places. A separator (coma or period) separates groups of three digits in real numbers greater than 999.

If the **1000 separator** is checked, then the number is shown in decimal format using the period and the commas. The characters recognized as numbers depend on the options you select in the Regional Settings of Control Panel. Fix mode sets the display to show the result with max 25-digit.

See also

Entering expression Basic calculations Molecular weight calculations Math and trigonometry functions Quadratic equation Statistical analyses

ANGLE MEASURE

Radian #rad

It is usual for scientists and engineers to measure angles in radians.

Radian is the angle at the center of a circle that intercepts an arc equal in length to the radius. From these definitions, it follows that 1 revolution = 4 right angles = 360° = 2pi radians.

Degree #deg

The word "degree" has many meanings in mathematics. The most common meaning is that it is the unit of Angle measure. This unit harks back to the Babylonians, who used a base sixty number system. Likely arises from the Babylonian year, which was composed of 360 days (12 months of 30 days each). The degree is subdivided into 60 Minutes per degree, and 60 Seconds per Minute.

Positive values move counterclockwise (that is, a line at 90° points straight up) and negative values move clockwise (a line at –90° points straight down)

If the values are greater than 360, then 360 is subtracted from them until the value is less than 360. (Entering an angle of 450° or 810° is the same as entering 90°). In other words, the angle is divided by 360 and the remainder is used as the angle.

Grade #grad

Grade is a unit of angular measure in which the angle of an entire Circle is 400 grads. A Right Angle is therefore 100 grads. A grade is sometimes also called a Gon or a Gradient.

The lines which started with # are command lines. With these lines it is possible to change the number format or the angle measurement. To change the measure angles into degrees, enter #deg in input line.

See also

Entering expression Basic calculations Molecular weight calculations Math and trigonometry functions

TROUBLESHOOT

Chemistry Assistant translates the texts into a mathematical expression and corrects the most common errors you encounter as you enter the expression into input line. The appearance of mathematical expression, which is the result of translation, can be seen if the mouse pointer is held over the tasks field.

Unknown chemical symbol

The program will try to translate the element symbols written in lowercase letters in the correct form. *Chemistry Assistant* will show the result of translation - or it will report an error.

R2O display R isn't element symbol!

Incorrect argument is entered

If an expression cannot properly evaluate a result, Chemistry Assistant will display an error value.

5/0 display Cannot divide by zero!

log-54 display Log of a negative number!

sqr-54 display Root of a negative number!

asin2 display Argument must be from -1 to 1

Incorrect syntax

Correct the syntax. Insert the correct mathematical syntax into the expression.

5***3 display Syntax error!

5*-*3 display Type mismatch

Match all open and close parentheses

Make sure all parentheses are part of a matching pair. You must not enclose arguments in parentheses 5*(15-6 display Missing right bracket ')' ! 15 6)*8 display Missing loft bracket '/' !

15-6)*8 display Missing left bracket '(' !

Enter all required arguments

Some functions have required arguments. Also, make sure you have not entered too many arguments. dat display No valid data!

Misspelling the name of a function

Correct the spelling. Insert the correct function name into the expression. When you an incorrect function name insert into the expression, the program will try to translate them into element symbol and show the result of translation - or it will report an error.

logr100 display R isn't element symbol!

Result is too large or too small

Entering an expression that produces a number that is too large or too small to be represented in *Chemistry Assistant* Change the expression so that its result is between –1E307 and 1E307

171! display Result is too large!

45⁴⁵⁰ display Overflow

The author will appreciate to hear your comments, suggestions and bugs you may encounter.

See also Entering expression Molecular weight calculations Math and trigonometry functions

INFO

Program:	EniG. Chemistry Assistant
Version:	1.8
Platform:	Win95/98/NT
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