

The Kalzium Handbook

Carsten Niehaus



The Kalzium Handbook

Contents

1	Introduction	1
2	Kalzium quick start guide	2
3	Using Kalzium	6
3.1	Overview of Kalziums usage	6
3.2	The information dialog	6
3.2.1	Overview	7
3.2.2	Picture	7
3.2.3	Bohr Orbitals	8
3.2.4	Chemical Data	9
3.2.5	Miscellaneous	10
3.2.6	Chemical Energies	11
3.2.7	Spectrum	12
3.3	Numeration	13
3.4	Color schemes	13
3.5	Tools	14
3.5.1	Nuclidboard	14
3.5.2	Nuclidboard	15
3.5.3	Glossary	15
3.5.4	Plot Data	16
3.5.5	Equation Solver	17
3.5.6	Sidebar	19
3.5.6.1	Overview	19
3.5.6.2	Calculate	20
3.5.6.3	Timeline	22
3.5.6.4	State of Matter	22
3.5.6.5	Show Legend	23

The Kalzium Handbook

4	Configuring Kalzium	24
5	Command Reference	27
5.1	Menus and shortcut keys	27
5.1.1	The File Menu	27
5.1.2	The View Menu	27
5.1.3	The Tools Menu	28
5.1.4	The Settings Menu	28
5.1.5	The Help Menu	29
6	Questions and Answers	30
7	How can I contribute?	31
8	Credits and License	32
A	Installation	33
A.1	How to obtain Kalzium	33
A.2	Requirements	33
A.3	Compilation and Installation	33

Abstract

Kalzium is a program which shows you the Periodic Table of Elements. You can use Kalzium to search for information about the elements or to learn facts about the periodic table.

Chapter 1

Introduction

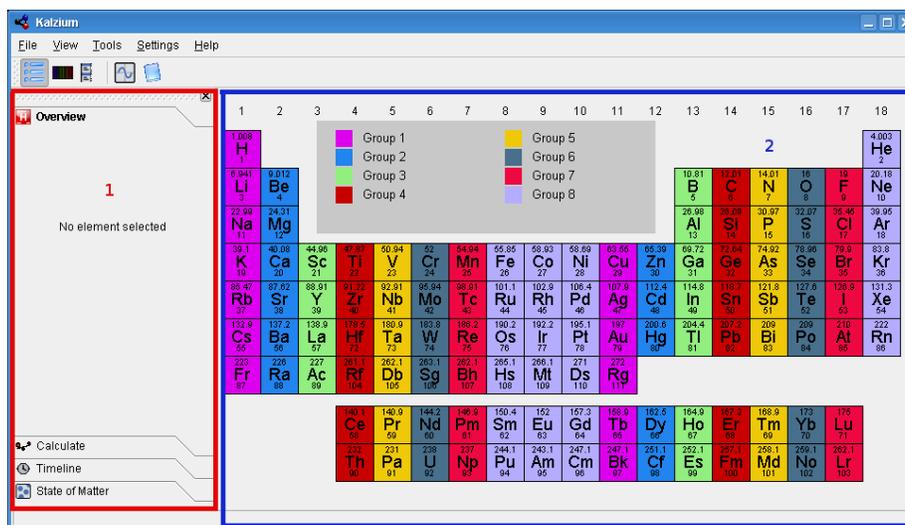
Kalzium provides you with all kinds of information about the Periodic Table of the Elements. You can lookup lots of information about the elements and also use visualizations to show them. It is free and licensed under the GNU Public License.

You can visualize the Periodic Table of the Elements by groups, blocks, acidic behavior, families, crystal structure or different states of matter. You can plot data for a range of elements for properties like the density or the atomic mass. You can go back in time and see what elements were known at a given date. You can also calculate the molecular mass of molecules.

Chapter 2

Kalzium quick start guide

Here is Kalzium the first time you run it, either from the K menu->Edutainment->Science->Kalzium or with Alt+F2 and entering **kalzium** into the field.



Kalzium is divided in a sidebar on the left (in red, 1) and the table view (in blue, 2) which shows the elements of the periodic table. The standard menubar allows you to choose what you want to display and the status bar reports facts. You can hide the sidebar using the View → Hide Sidebar menu.

When you move the mouse cursor on an element of the table, a tooltip appears with a picture of this element if available, its number and its mass. In the sidebar is displayed an overview of the current element in the Overview tab.

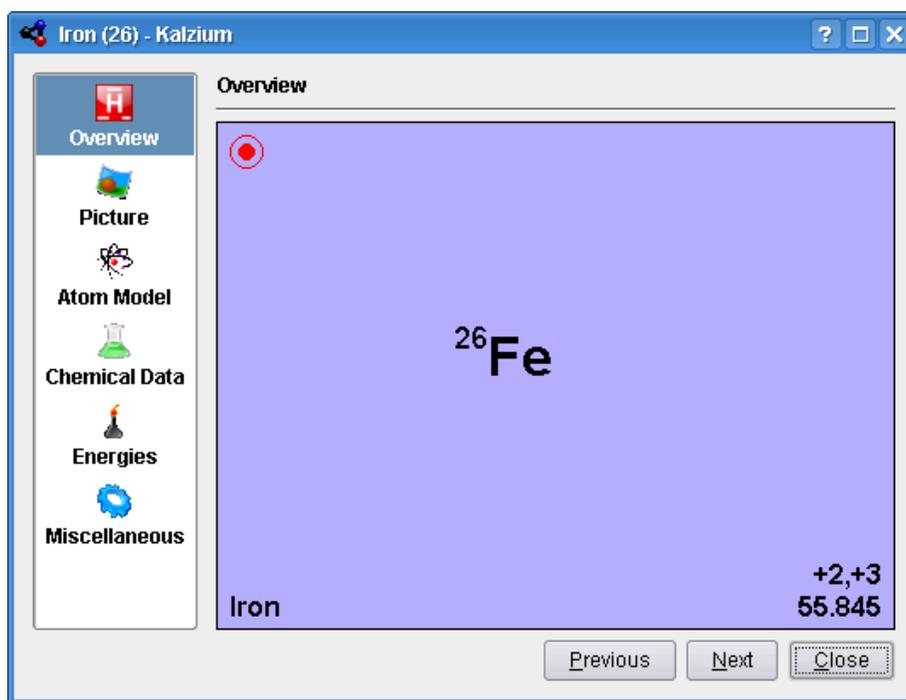
You can disable the tooltips using the View → Hide tooltip menu.

You can choose several views for the table: display the elements per families,

The Kalzium Handbook

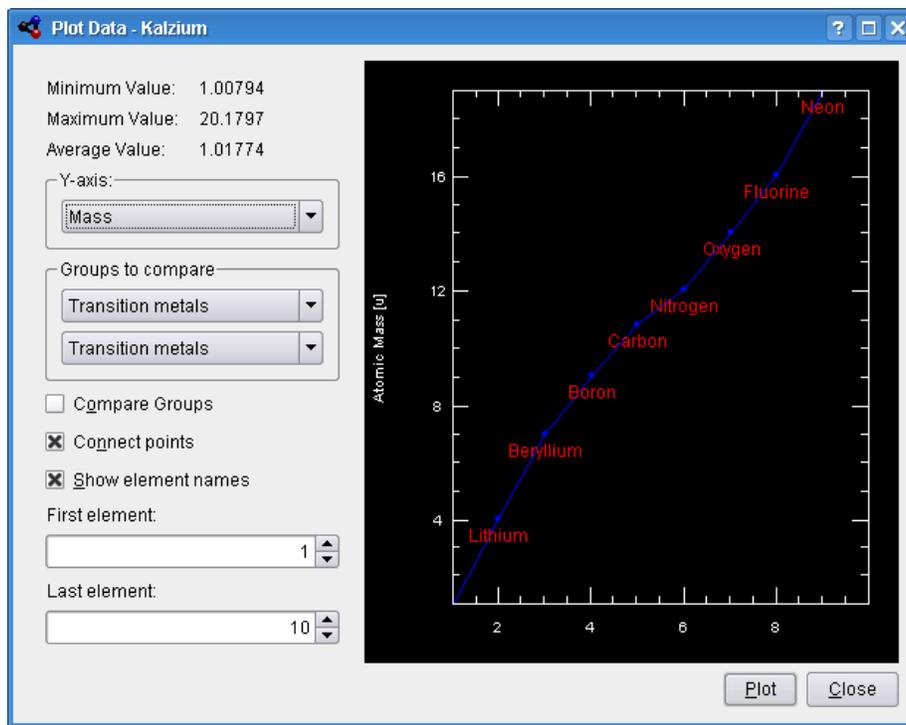
per groups, per crystal structure, depending on their acidic behaviour, etc.. You can change all that in the menubar in the View → Look menu.

If you want to know facts about a precise element, click on it in the table and the information dialog will be displayed.



You can plot data using the Tools → Plot Data menu. You choose what you want to plot on the y-axis and a range of elements to plot taht for on the x-axis. The screenshot below shows the mass of the elements 1 to 10.

The Kalzium Handbook



The Glossary (Tools → Glossary) explains the most important chemical words and shows you pictures of the most common tools along with an explanation.

The Kalzium Handbook

Glossary - Kalzium

Search:

- Full Pipette
- G
 - Graduate
- H
 - Heating Coil
- L
 - Litmus Paper
- M
 - Magnetic stir bar**
 - Magnetic Stir Bar Retriever
 - Mortar
- P
 - Pileusball
 - Pipette
 - Protective Goggles
- R
 - Reflux Condenser
 - Refractometer
 - Rotary Evaporator
 - Round-bottomed Flask
- S
 - Scales
 - Separating Funnel
 - Separation Beaker
 - Short-stem Funnel

Magnetic stir bar



Magnetic stir bars are highly chemically inert, small magnetic bars. Most heaters have a built-in magnet which can rotate. Through this rotation the magnetic stir bars are spun and the solution the magnetic stir bar is in is homogenized.

Close

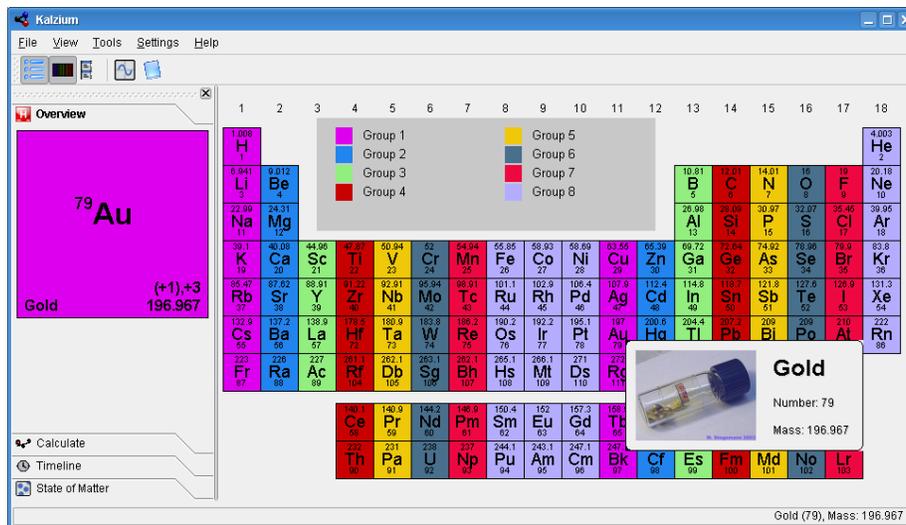
Chapter 3

Using Kalzium

3.1 Overview of Kalziums usage

Here are some screenshots of Kalzium in action:

Kalzium is very easy to use. It is specially designed for students of all ages to use as a small and quick database.



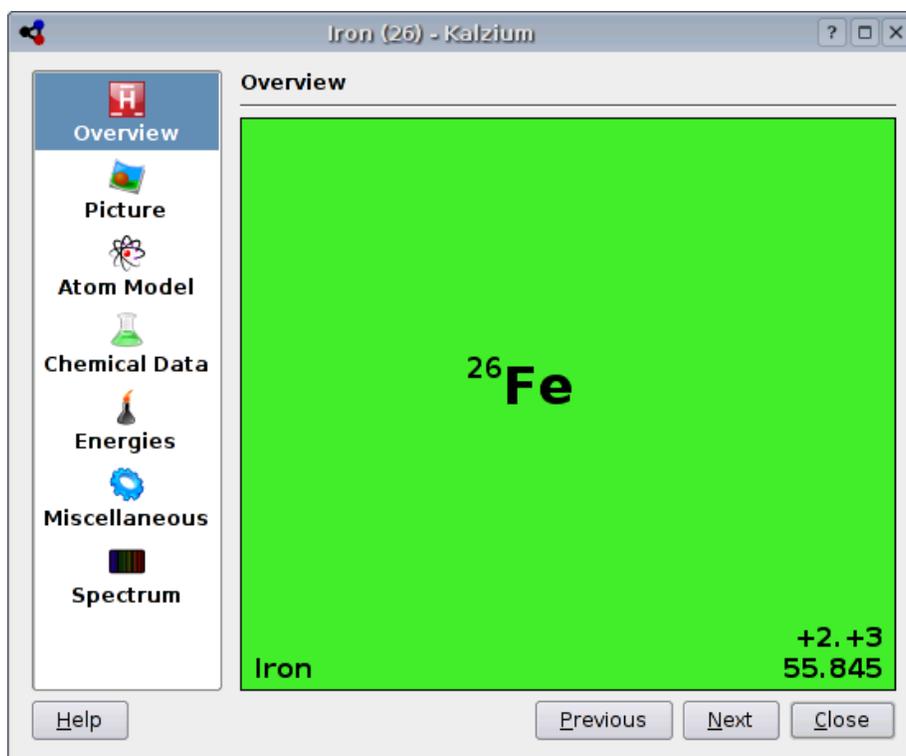
3.2 The information dialog

The information dialog is accessed by clicking with the left mouse button on any element. It is available only in the Overview mode or when the sidebar is

hidden. This is the place to get information about an element. With the buttons at the bottom of the dialog or with the use of the mousewheel you can change the element which is displayed without closing the dialog.

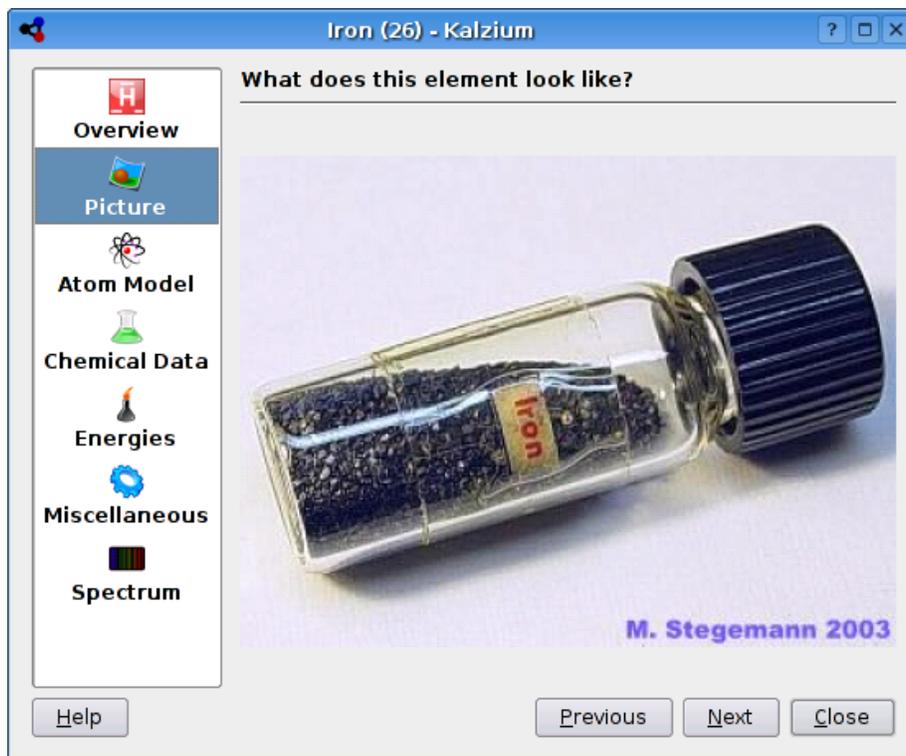
3.2.1 Overview

In the Overview you will find the most important information about the element. In the middle you see the symbol of the Element with it's elemental number in the top left. The bottom-left corner displays the name of the element while the bottom-right corner shows the most important oxidation-stages and, below that, the elemental weight



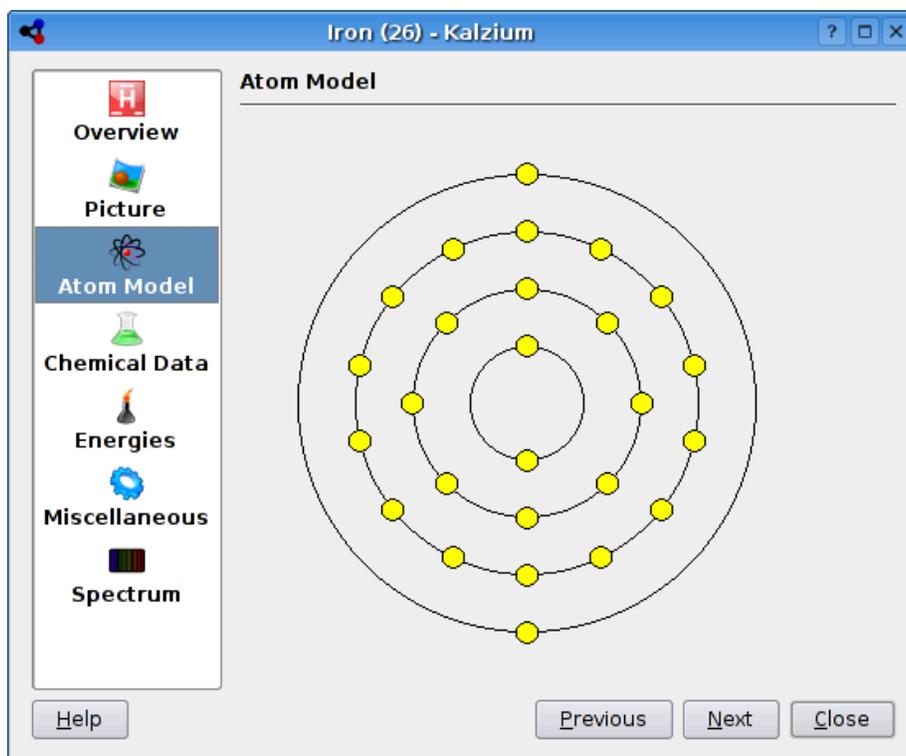
3.2.2 Picture

The Picture tab displays a picture of the element when available.



3.2.3 Bohr Orbitals

The Atom Model tab displays the atomic shells. Every orbit stands for a atomic shell and every yellow circle represents an electron.



3.2.4 Chemical Data

The Chemical Data tab presents some atomic data. The first entry is the Orbital structure. The next is the density.

Depending on the data available in Kalzium you will see different radii of the element. The covalent radius is the radius of a non charged atom of the element in a molecule. The could for example be the O-H-distance in Water. The atomic radius is the radius of an elemental atom, e.g. not bound to anything. The van der Waals-radius is defined as the distance of two atoms of the same sort in two equal molecules, for example two carbon-atoms in propane. The last possible radius is the ionic radius including its charge.

The mass of an element is the avarage mass of all isotopes in relation to their percentage.

Some elements have information about their isotopes.

Mass The mass of this isotope.

Neutrons The number of neutrons this isotope has.

The Kalzium Handbook

Percentage The percentage of atoms occurring that are of this isotope type. Also called abundance.

Half-life period Only unstable isotopes have a half-life period. It is defined as the time in which half the isotopes decay.

Energy and Mode of Decay Some isotopes are known to emit particle radiation under the process of radioactive decay. Each decay transformation has a typical energy release, which is listed along with the mode of decay.

Spin and parity The spin of the nucleus and its parity.

Magnetic Moment The magnetic dipole moment of the nucleus. Measured in units of the nuclear magneton.

Iron (26) - Kalzium

Chemical Data

Fe Block: d

Orbital structure: $Ar\ 3d^6\ 4s^2$

Density: $7.874\ g/cm^3$

Covalent Radius: $124.1\ pm$

Atomic Radius: $140\ pm$

Mass: $55.845\ u$

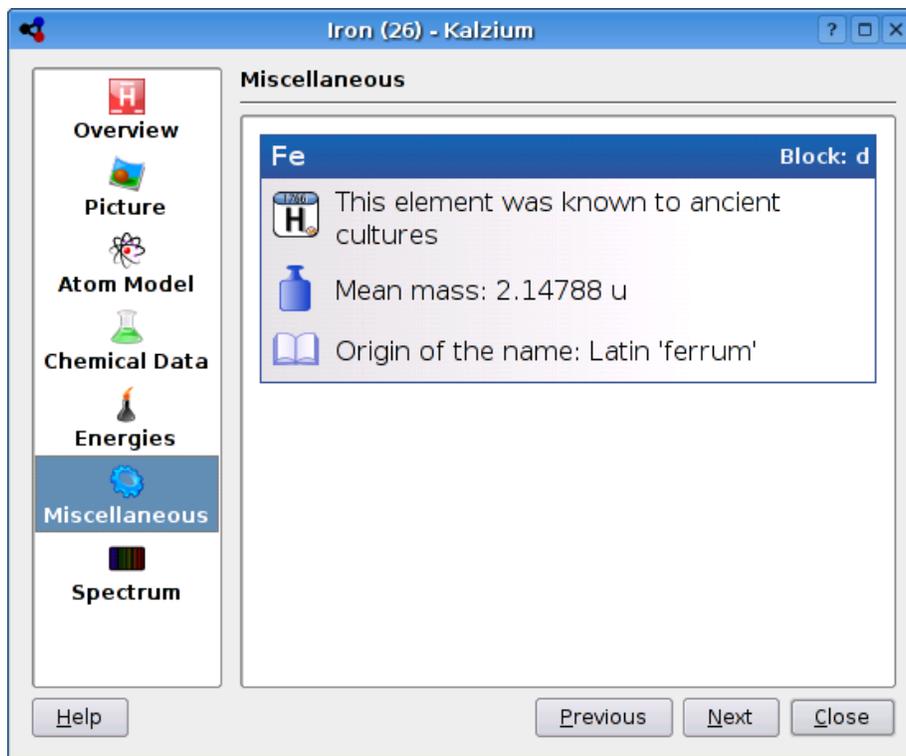
Isotope-Table						
Mass	Neutrons	Percentage	Half-life period	Energy and Mode of Decay	Spin and Parity	Magnetic Moment
$53.94\ u$	28	5.81%			$0+$	$0\ \mu_n$
$55.935\ u$	30	91.64%			$0+$	$0\ \mu_n$
$56.935\ u$	31	2.21%			$1/2-$	$+0.090623\ \mu_n$
$57.933\ u$	32	0.34%			$0+$	$0\ \mu_n$

Help Previous Next Close

3.2.5 Miscellaneous

The Miscellaneous tab tells you other informations about the current element, including when it was discovered, its mean mass (the mass per neutron) and the origin of the name.

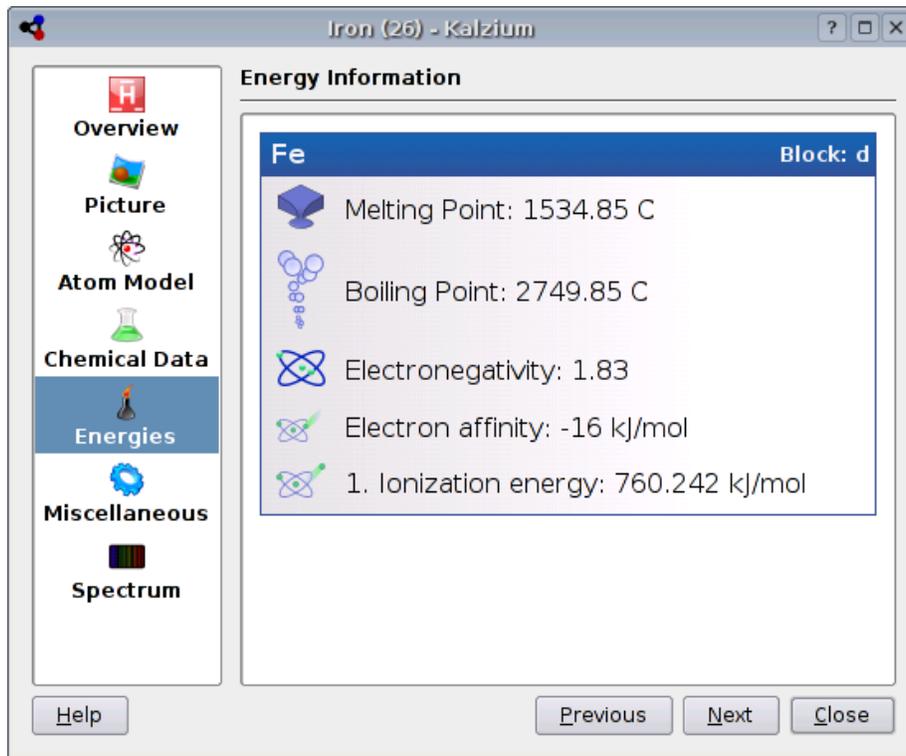
The Kalzium Handbook



3.2.6 Chemical Energies

The Energies tab tells you about different energy facts related to the element.

The Kalzium Handbook

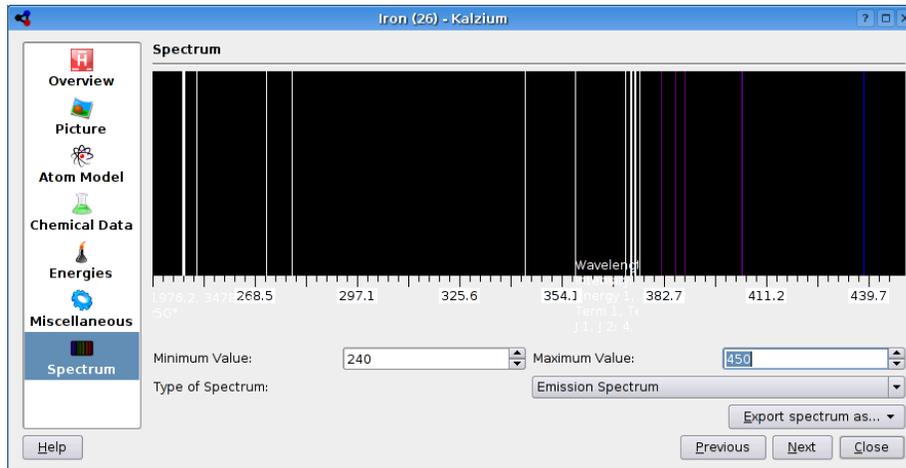


The screenshot shows the 'Energy Information' window for Iron (Fe) in the Kalzium software. The window title is 'Iron (26) - Kalzium'. On the left is a sidebar with navigation options: Overview, Picture, Atom Model, Chemical Data, Energies (selected), Miscellaneous, and Spectrum. The main area displays the following data for Fe (Block: d):

- Melting Point: 1534.85 C
- Boiling Point: 2749.85 C
- Electronegativity: 1.83
- Electron affinity: -16 kJ/mol
- 1. Ionization energy: 760.242 kJ/mol

At the bottom of the window are buttons for 'Help', 'Previous', 'Next', and 'Close'.

3.2.7 Spectrum



The screenshot shows the 'Spectrum' window for Iron (Fe) in the Kalzium software. The window title is 'Iron (26) - Kalzium'. The left sidebar is the same as in the previous screenshot, with 'Spectrum' selected. The main area displays a line spectrum with several vertical lines of varying colors (black, purple, blue, green, yellow, red) on a black background. The x-axis is labeled 'Wavelength' and has numerical markers at 197.6, 247, 268.5, 297.1, 325.6, 354.1, 382.7, 411.2, and 439.7. Below the spectrum, there are controls for 'Minimum Value' (set to 240), 'Maximum Value' (set to 450), and 'Type of Spectrum' (set to 'Emission Spectrum'). There is also an 'Export spectrum as...' button and 'Previous', 'Next', and 'Close' buttons at the bottom.

3.3 Numeration

The numeration is the way of numbering the 18 groups of the periodic table. You can change the numeration to IUPAC, old IUPAC or CAS, or you can switch it off entirely.

The following options in the View Numeration menu can be used to change the numeration shown:

- No Numeration: if this option is active, no period-numeration will be in effect.
- Show IUPAC (default): the IUPAC is the *International Union of Pure and Applied Chemistry*. This is an organization which defines most of the standards for chemical concerns. The new IUPAC system numbers each column with Arabic numbers from 1 (one) through 18 (eighteen).
- Show CAS: the CAS is the *Chemical Abstracts Service*. In the CAS system the letters A and B were designated to main group elements (A) and transition elements (B). Though the IUPAC numeration is the official, the CAS numeration is what is still used in classrooms and laboratories.
- Show Old IUPAC: the old IUPAC system labeled columns with Roman numerals followed by either the letter 'A' or 'B'. Columns were numbered such that columns one through seven were numbered 'IA' through 'VIIA', columns 8 through 10 were labeled 'VIII A', columns 11 through 17 were numbered 'IB' through 'VIIB' and column 18 was numbered 'VIII'. Because of the confusion the old IUPAC and the CAS system created, the IUPAC adopted their new system.

3.4 Color schemes

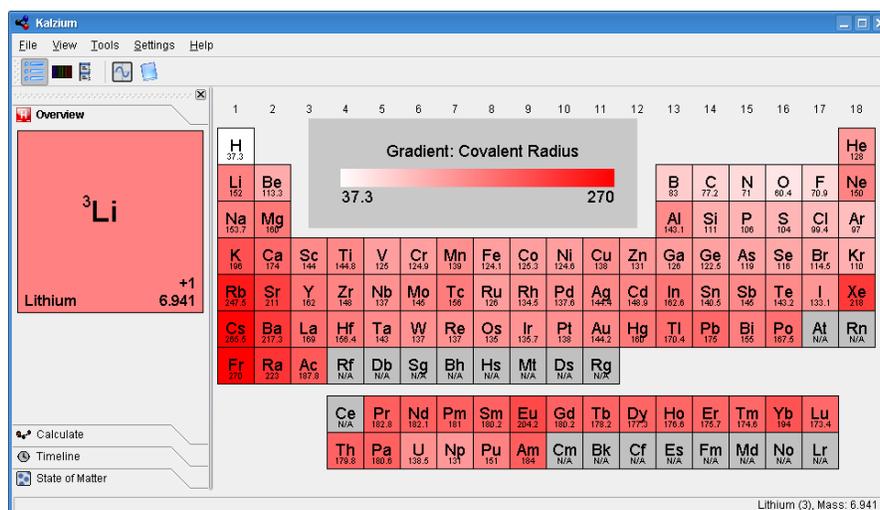
Kalzium can show you which elements are where with regard to their Periodic 'block' and 'group', their behavior with acid and which state of matter (i.e. solid/liquid/vapor) they are in at a given temperature.

Color schemes can be changed in the View Look menu.

- No Color Scheme: all the elements have the same color. You can change the default color by choosing Settings → Configure Kalzium... and going to the Colors tab.
- Show Groups: displays a color for each group. A group is a vertical column in the periodic table of the elements. There are 18 groups in the standard periodic table. Elements in a group have similar configurations of their valence shell electrons, which gives them similar properties.
- Show Blocks: displays a color for each block.
- Show Acid Behavior: represents each acidic behaviour with a different color.

The Kalzium Handbook

- Show Family: represents each of the nine families with a color.
- Show Crystal Structures: colors each element depending on its crystal structure.
- Gradient
The gradient views displays the elements according to a property you can select below and with a gradient colored scheme. The elements for which the data is not available are displayed in grey.



- Atomic Radius
- Covalent Radius
- van der Waals Radius
- Atomic Mass
- Density
- Boiling Point
- Melting Point
- Electronegativity
- Electron Affinity

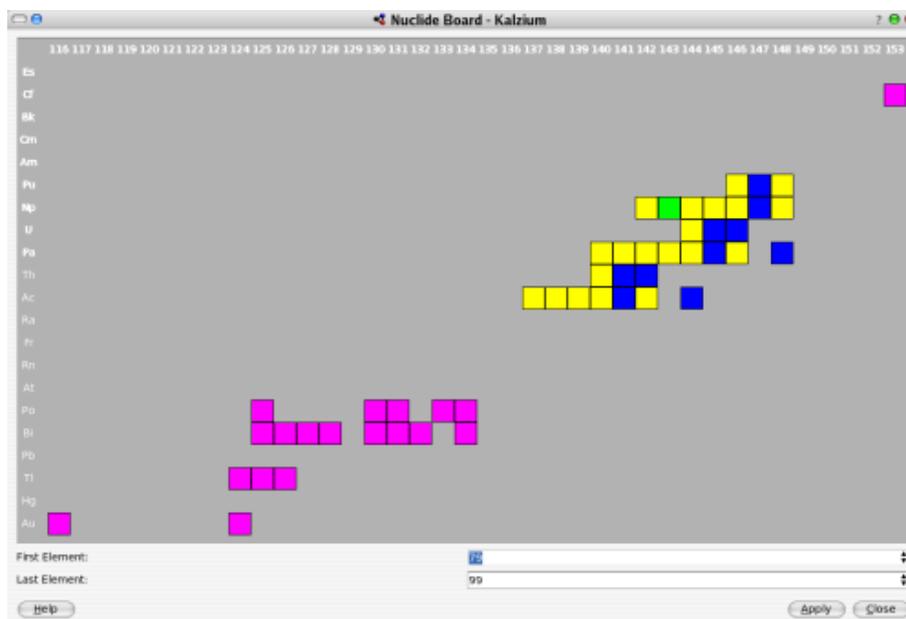
3.5 Tools

3.5.1 Nuclidboard

The Nuclidboard shows you the isotopes of the elements.

The dialog shows the element number on the y-axis. The x-axis displays there are different kinds of isotopes, some are stable, some are not. The unstable isotopes can decay as alpha-rays or two different beta-rays. These differences are encoded by using different colors.

The Kalzium Handbook



Kalzium can display the isoptes of a range of elements

3.5.2 Nuclidboard

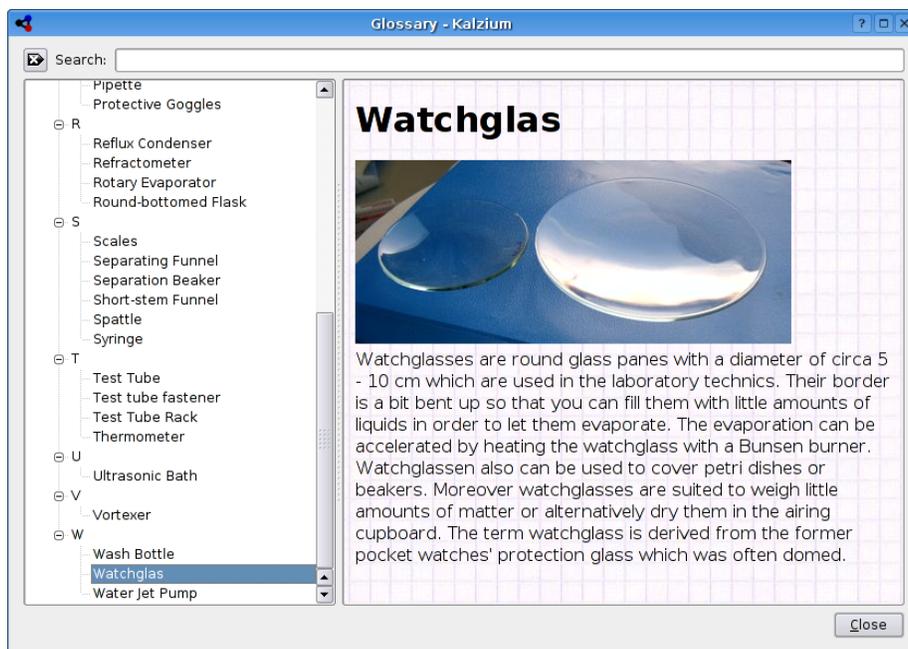
The R/S Phrases blah blah

3.5.3 Glossary

The Glossary gives you definitions of the most used tools in chemistry as well as some knowledge data. On the left side of the windows you can see the tree of items. On top, there are chemical terms, below that there is a second tree of laboratory-tools.

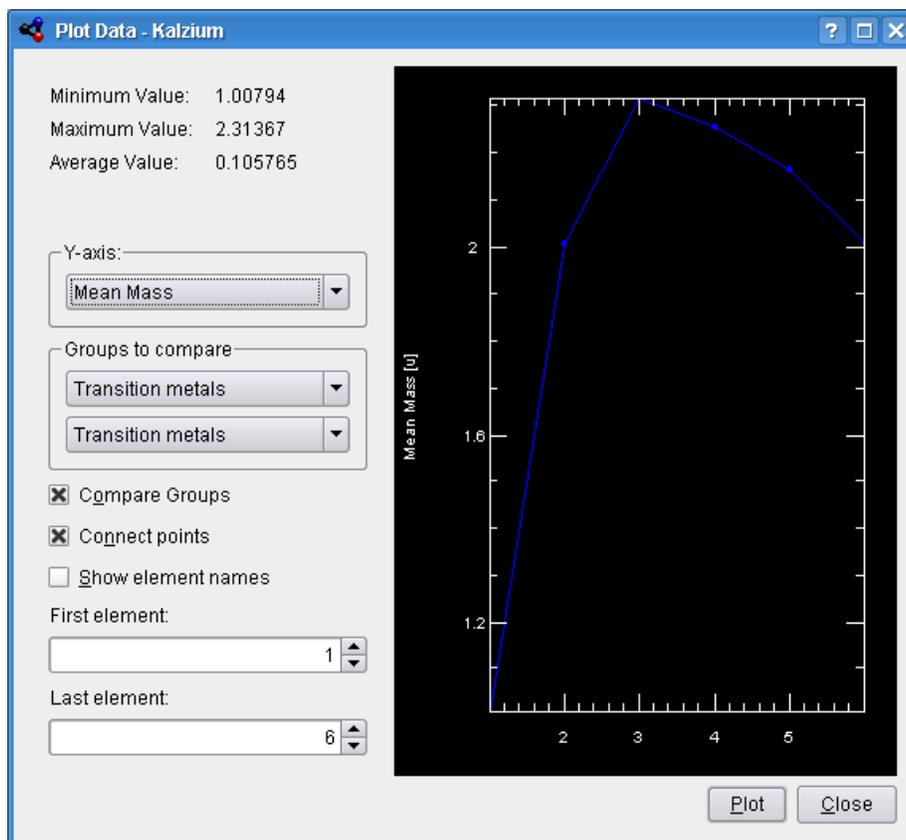
On the top of the widget you can see a searchbar. If you type in the bar the trees will be adjusted immediately. The small button left of the searchbar will clear it.

The Kalzium Handbook



3.5.4 Plot Data

The Plot Data dialog allows you to plot some information about elements. The X-axis represents a range of elements (from one number to a higher number). You set this range using the First Element and Last Element fields on the dialog. The display does not change until you click on the Plot button.



Kalzium can plot some data about a range of elements.

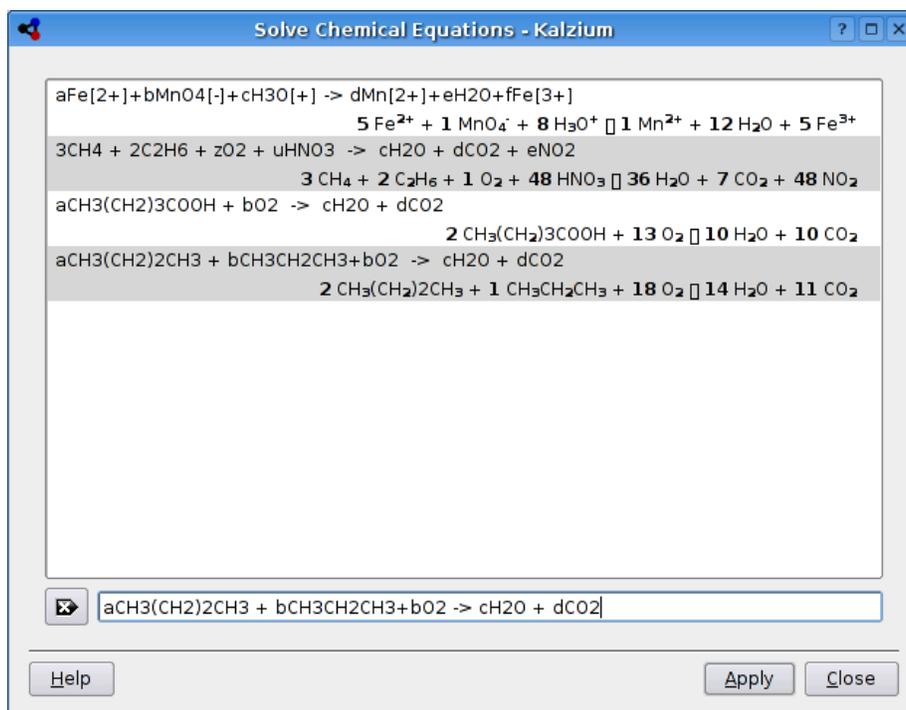
3.5.5 Equation Solver

The Equation Solver enables the user to solve chemical equations. This is an example:



The computed equation will be displayed on the right side of the window. As you can see in the first example you can also define the value of one or more coefficients. The other coefficients will be adjusted. Furthermore, it is possible to use brackets around elements or electronic charges as shown in the last two examples.

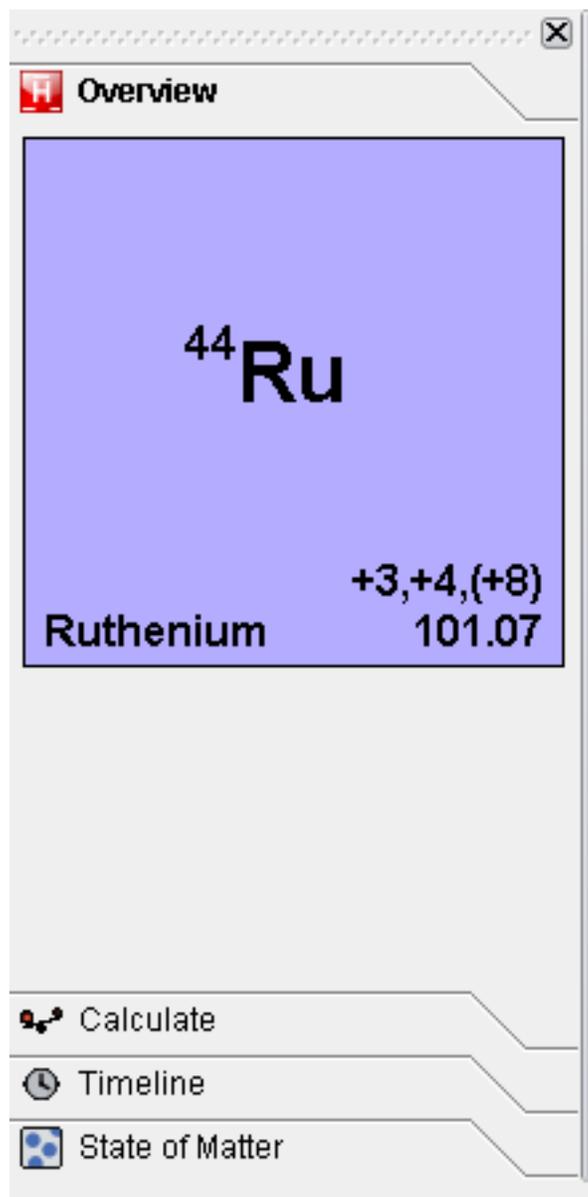
The Kalzium Handbook



Kalzium can solve chemical equations

3.5.6 Sidebar

3.5.6.1 Overview



The Overview tab is the first one and it shows you an overview of the element the mouse is over.

3.5.6.2 Calculate

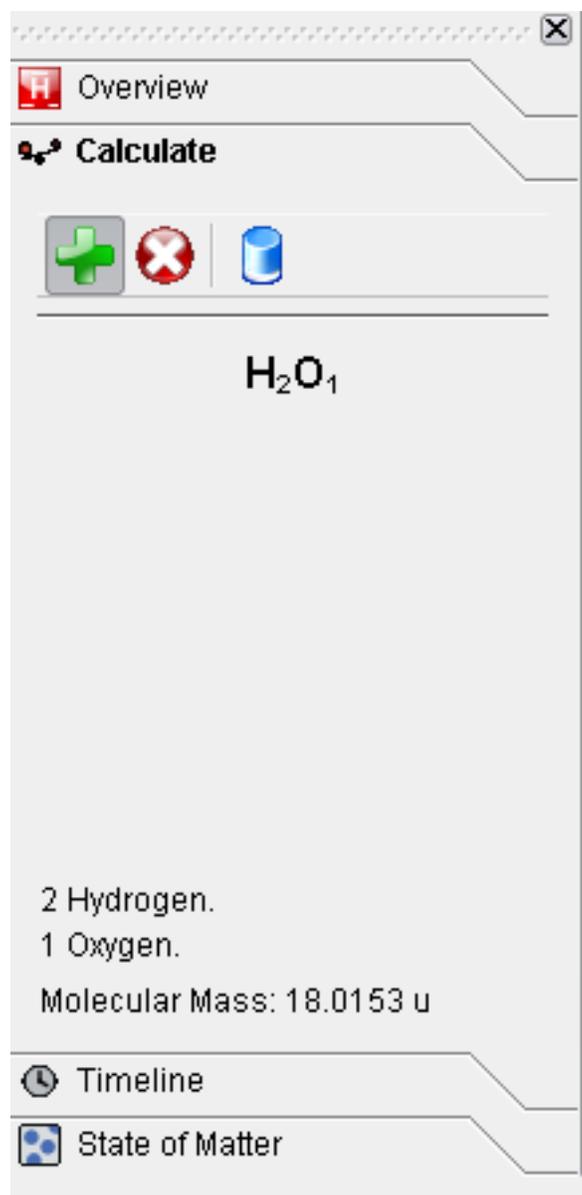
The Calculate tab is the second in the sidebar. It allows you to calculate molecules weights.

You are first presented with the following icons and text:



Calculate

You have to click on the elements that compose the molecule.



Weight

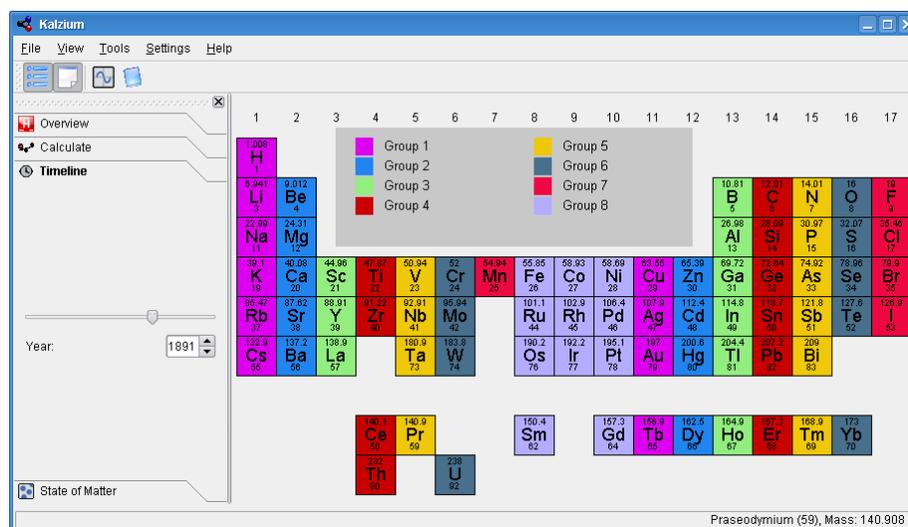
You can remove some elements after you click on the Remove icon. You can also clear all the elements with the Clear icon on the most right.

3.5.6.3 Timeline

The Timeline feature allows you to explore the elements of the set time period. This is great for getting a feel for how the PSE evolved over time, as more and more elements were discovered. If you move the slider you will notice that some elements disappear if you move it to the left and reappear if you move it to the right. Furthermore the number will change constantly.

The number represents the date you are looking at. If you move the slider to e.g. 1856 you will only see the elements which were known in the year 1856.

You will notice that some elements are not even shown in the current year. This is because some of the elements have not been discovered yet but are predicted to exist.

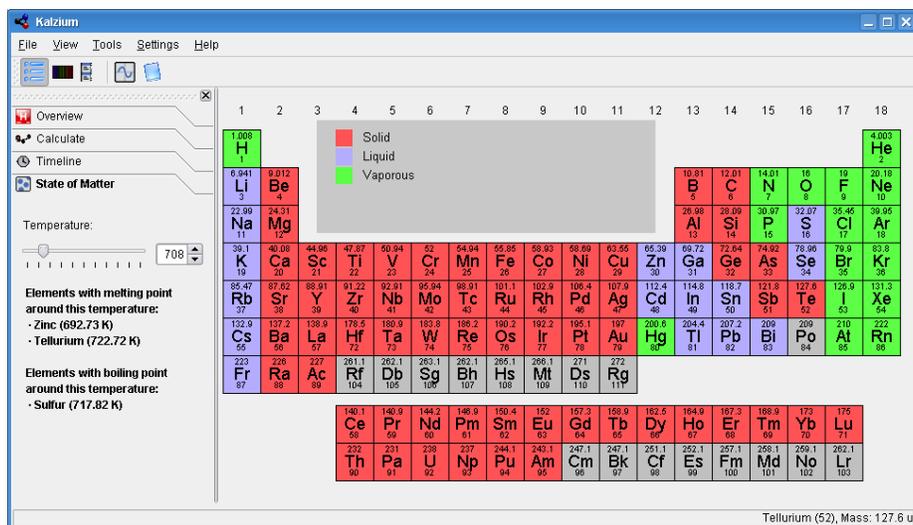


The PSE back in time (elements known in 1856)

3.5.6.4 State of Matter

With the State of Matter function, you can choose a temperature and view the state of each element at that temperature. You can easily visualize how many elements and what elements are, for example, solid at a given temperature. So you can learn that almost all are solid at very low temperatures and that most are liquid or even vaporous at high temperatures.

The Kalzium Handbook



Kalzium can show you which elements are solid/liquid/vaporous at a given temperature.

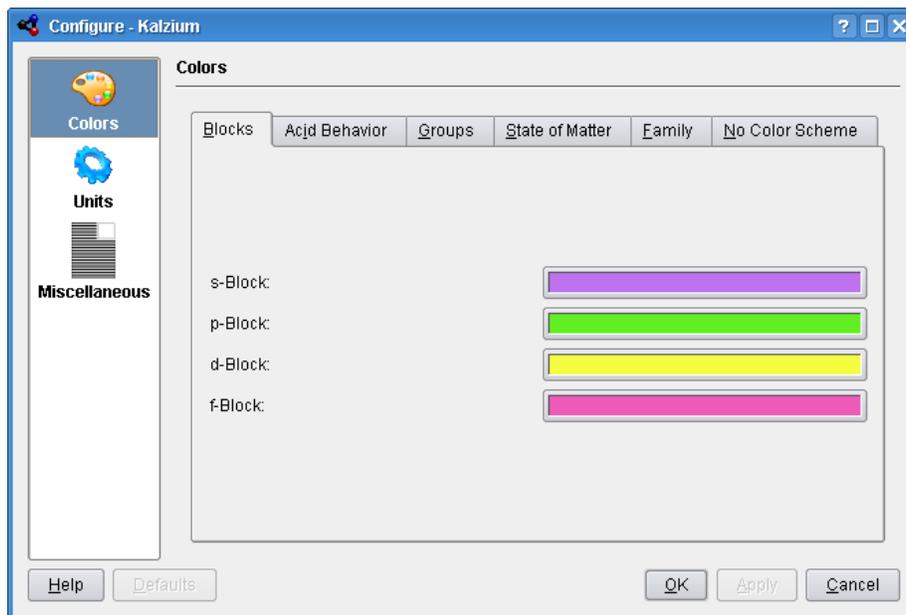
3.5.6.5 Show Legend

The Show Legend action allows you to display the legend for the scheme you are in (Groups, Blocks, Acid Behavior). The legend is displayed by default but if you hide it, it will stay hidden until you choose to show it. Kalzium will keep this setting in its configuration file, so that the next time you run it, the setting will be as you left it.

Chapter 4

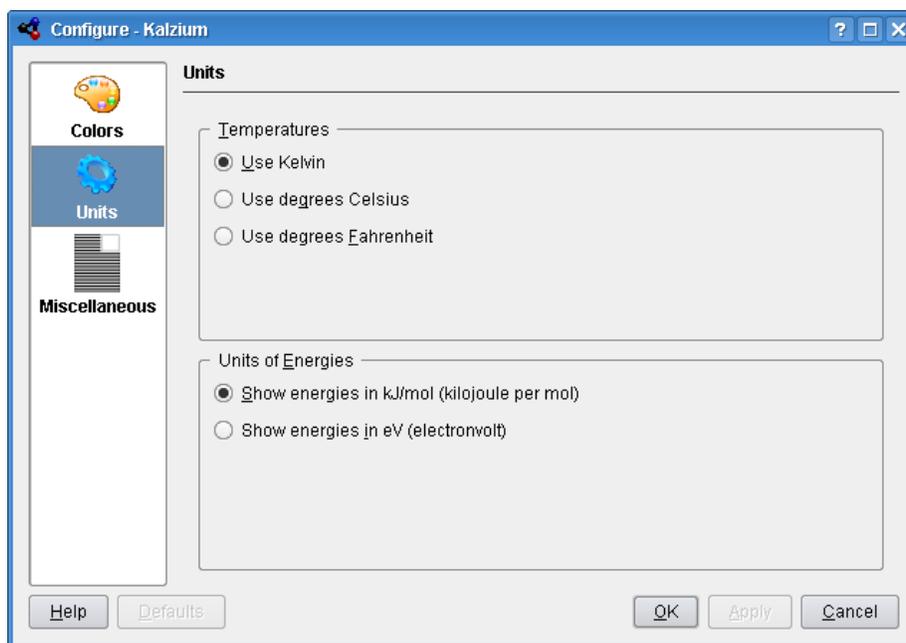
Configuring Kalzium

Kalzium has many configuration options, which you can access by opening the configuration dialog by selecting Settings → Configure Kalzium... from the menu.



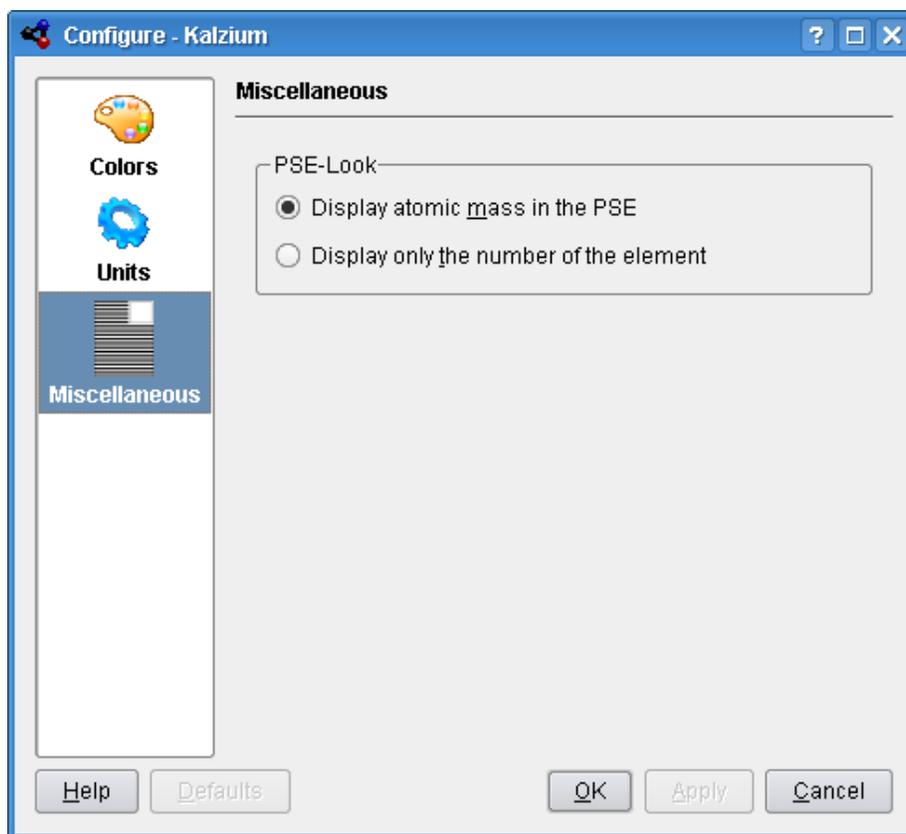
In the Colors tab, you can change the different colors for each scheme.

The Kalzium Handbook



In the Units tab, you can choose the units. You can select if you prefer kJ/mol by default or you can choose eV. The Temperature is in Kelvin by default but you can change to degrees Celsius or degrees Fahrenheit.

The Kalzium Handbook



In the Miscellaneous tab, you can find other options not related with the previous tabs.

Chapter 5

Command Reference

5.1 Menus and shortcut keys

5.1.1 The File Menu

File → Quit (Ctrl+Q) Quits Kalzium

5.1.2 The View Menu

View → Numeration → No Numeration Display no numeration scheme

View → Numeration → Show IUPAC Display the IUPAC numeration

View → Numeration → Show CAS Display the CAS numeration

View → Numeration → Show Old IUPAC Display the Old IUPAC numeration

View → Look → No Color Scheme Display no color scheme

View → Look → Show Groups Display the groups of elements

View → Look → Show Blocks Display the four blocks of elements

View → Look → Show Acid Behaviour Display the acidic behaviour

View → Look → Show Families Display the families of elements

View → Look → Show Crystal Structures Display crystal structures

View → Look → Gradient → Atomic Radius Display the elements atomic radius

The Kalzium Handbook

View → Look → Gradient → Covalent Radius Display the elements covalent radius

View → Look → Gradient → van der Waals Radius Display the elements van der Waals radius

View → Look → Gradient → Atomic Mass Display the elements atomic radius

View → Look → Gradient → Density Display the elements atomic radius

View → Look → Gradient → Boiling Point Display the elements boiling point

View → Look → Gradient → Melting Point Display the elements melting point

View → Look → Gradient → Electronegativity Display the elements electronegativity

View → Look → Gradient → Electron Affinity Display the elements electron affinity

View → Show Legend Toggle the legend view

View → Show/Hide Tooltip Toggle tooltip display on elements

View → Show Sidebar Toggle the Sidebar

5.1.3 The Tools Menu

Tools → Plot Data Open the Plot Data dialog

Tools → Nuclide Board Open the Nuclide Board dialog

Tools → Glossary Open the Glossary

Tools → R/S Phrases Open the R/S Phrases dialog

Tools → Show Equationsolver Open the Equationsolver dialog

5.1.4 The Settings Menu

Settings → Show Toolbar Toggle the Main Toolbar

Settings → Show Statusbar Toggle the Statusbar

Settings → Configure Shortcuts... Configure the keyboard keys you use to access the different actions.

Settings → Configure Toolbars... Configure the items you want to put in the toolbar

Settings → Configure Kalzium... Display the Kalzium settings dialog

5.1.5 The Help Menu

Help → **Kalzium Handbook (F1)** Invokes the KDE Help system starting at the Kalzium help pages. (this document).

Help → **What's This? (Shift+F1)** Changes the mouse cursor to a combination arrow and question mark. Clicking on items within Kalzium will open a help window (if one exists for the particular item) explaining the item's function.

Help → **Report Bug...** Opens the Bug report dialog where you can report a bug or request a 'wishlist' feature.

Help → **About Kalzium** This will display version and author information.

Help → **About KDE** This displays the KDE version and other basic information.

Chapter 6

Questions and Answers

1. *Will I ever have to pay for Kalzium?*

No, never. But the author always welcomes a nice mail or a DVD as a 'Thank You'. Kalzium is licensed under the [GPL](#), so you will never have to pay for this program.

2. *Will there ever be a Windows® version?*

No, at the moment not, but you can download the source and make your own Windows® version. It should not be a big problem, because it is written with Trolltech Qt™ libs. But what do you need Windows® for? Get the latest Linux®, and live on the edge.

Chapter 7

How can I contribute?

1. *Support me with data.*

In the world of science, the progress is quite fast. If you ever find an incorrect or missing value, please drop me an email.

2. *Find some bugs or give some suggestions*

If you find any bugs in the program, or have a few suggestions for improvements, please let me know at cniehaus@kde.org.

Chapter 8

Credits and License

Kalzium

Program Copyright, 2001-2005 Carsten Niehaus cniehaus@kde.org

Contributors:

- Pino Toscano toscano.pino@tiscali.it

This documentation is licensed under the terms of the [GNU Free Documentation License](#).

This program is licensed under the terms of the [GNU General Public License](#).

Appendix A

Installation

A.1 How to obtain Kalzium

Kalzium is part of the KDE project <http://www.kde.org/> .

Kalzium can be found in the kdedu package on <ftp://ftp.kde.org/pub/kde/> , the main FTP site of the KDE project.

A.2 Requirements

Kalzium itself can be found on [The Kalzium home page](#) and is part of the KDE-Edu project

You can find a list of changes in the file `ChangeLog` in the distribution of Kalzium.

A.3 Compilation and Installation

In order to compile and install Kalzium on your system, type the following in the base directory of the Kalzium distribution:

```
% ./configure
% make
% make install
```

Since Kalzium uses **autoconf** and **automake** you should have no trouble compiling it. Should you run into problems please report them to the KDE mailing lists.