Ural Chemical Calculator Help Content

Ðóññêèé

Ural Chemical Calculator - what is it?

Ðóññêèé

This program has been designed to calculate the masses of the starting substances and of respective products of chemical reactions. The reaction equation may be exactly or only partially known. The program features include:

- supported and easy to edit database of chemical compounds;
- automatic calculation of the mole masses of the compounds;
- automatic control of the reaction equation;
- automatic calculation of the coefficients of the reaction equation;
- use of the reagents and products in the calculation either as individual substances or as mixtures with other compounds. The component concentration can be expressed in any form used in chemistry;
- the output of calculation results to printer or to other WINDOWS applications (Word, Excel etc.).

The program saves time and significantly decreases the chance of mechanical errors.

Using UrChemCalc involves the following steps:

- Input or edit equation of chemical reaction (in the main window),
- input required mass of one of the components (program will calculate other masses),
- output results.

UrChemCalc is the shareware product (it requires the registration for legal use).

Main window of Ural Chemical Calculator

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The main window contains a table with columns, which consist of fields of different kinds:

- numeric fields of reaction coefficients (may or may not be integers). A few of them (or all) may be fixed and shaded with aqua color. Others are calculated automatically, if the switch Autocalculation of coefficients is turned on;
- fields of compound names for reagents (in the left half of the window) and products (in the right part). One can choose these names from the compound database by clicking buttons with arrows;
- numeric fields of masses, one of which (selected manually) shaded with yellow color. Other fields are calculated automatically.

In the bottom part of main window are (from left to right): the material balance indicator (Balance_Ok/NOT_FULL), the switch for Autocalculation of coefficients, and (if this switch is turned on) the solution indicator. In the top part of main window the menu for access to the following program options is located:

- **Language**- choices of program interface language;
- **Database** - edit chemical compound database;
- **Output** - the output of calculation results to a printer or other WINDOWS applications (Word, Excel etc.) with preview on the screen;
- **Reset** - clears all the fields in main window to prepare for new equation input;
- **Help** - call:
    - local UrChemCalc Help,
    - window with short information **about** program,
    - UrChemCalc **Home Page** in World Wide Web (if the WWW-browser is found),
    - message **to developer** composer (also via WWW),
    - registration window (if the copy is not registered);
- **Exit** - closes the main window and terminates the program.

In addition, the main window contains standard WINDOWS components - sizing buttons, close (or system menu) button and window header with the program name and the version number.

See also Input the chemical reaction equation

The chemical compound database

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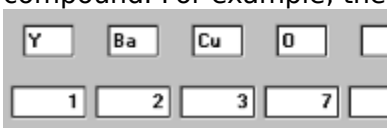
The database (files OUR.*) may be edited in two ways:

- choosing the phrase "New compound" from the list in the name field (Main Window). In this case one can add new database record;
- clicking the **Database** item in the main menu (Main Window). In this case all database records are available for editing or deleting. One can add records also. Open window contains the list of compound names. It may be used to move from one record to another as well as edit compound name in the list. The current record is shaded by a specific color. Several pairs of fields (element-coefficient) of the current record are under the list of names. The values in the fields must correspond to the chemical composition of the compound. For example, the compound YBa2Cu3O7 may look as:



The coefficients need not necessarily be integer (solid and liquid solutions, non-stoichiometric compounds, etc.). However, following is advisable:
- make a name corresponding to values in the fields of elements and coefficients;
- do not use a name twice;
- do not use "New compound" as a compound name.

If the name field is empty after record editing, the program will compose a name from element symbols and numbers in respective fields. On the contrary, if these fields are empty and the name field is not empty, the program will try to compose the record from the name. If the database contains a record with the same name, UrChemCalc reports this fact.

UrChemCalc provides a user with simplest method to fill the name field by clicking the button  . In this case, the program will compose the name from element symbols and numbers set in respective fields. The button  , on the contrary, composes the current record from the name. The button  evokes Solution Wizard. Be careful - the wizard will edit the current record! If the solution must be in a new record, dont forget to click the button **Insert** to make a new place!

The Periodic Table is evoked by double clicking on the element field or by the popup menu of this field. Then, you can choose the desirable element to be placed in the field. The mole mass field in the right part of the window is a calculated filed and cannot be edited. However you can copy this field in Clipboard and use the copy in other programs.

Double clicking the coefficient field enables you to divide all coefficients of the current record by some number. This procedure keeps proportions between elements more accurately than manual editing of coefficients.

In the bottom part of the window the following buttons are found:

Ok - save last changes, close the window and switch on the main window;
Cancel - cancel last changes of the current record, close the window and switch on the main window;
Help - call UrChemCalc Help;
Insert - add a new database record. After that you may begin the editing it;
Delete - delete the current record. The confirmation will be requested.

The chemical element database

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This database (files mendelev.*) is very important correct functioning of the program. It contains the information about atomic weight, notation, place in Periodic Table, etc. for all chemical elements. Do not edit this database unless absolutely necessary!

Output

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The Main Window menu has the item **Output**, which opens the result output preview window. The **Format** item in the preview window allows for selection of output format. All changes are reflected in the window at once, so these options do not need a detailed description. The window images scale (not that for hard copy!) can be changed clicking the **Preview scale** item. You can send results to a printer (by the **Output\Print** item) or copy it into WINDOWS Clipboard in the different formats (**Output\Text**, **Output\MS_Word**, **Output\Text_for_MS_Excel**). These options are available only for registered copies of Ural Chemical Calculator.

The **Close** item returns Main Window.

Ââîä óðàâíåíèÿ õèìè÷åñêîé ðåàêöèè

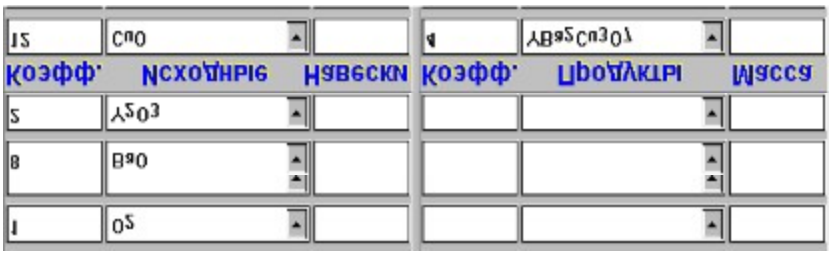
English

Óðàâíåíèå ðåàêöèè â ïðîãðàììå "Õèìè÷åñêèé êàëüêóëÿòîð" ðàñïîëàãàåòñÿ â ãëàâíîì îêíå è âûãëÿäèò íåñêîëüêî íåïðîñòî. Ãðóïïû ïî òðè êîëîíêè ñîîòâåòñòâóþò: ëåâàÿ - èñõîäíûì âåùåñòâàì, ïðàâàÿ - ïðîäóêòàì ðåàêöèè. Êàæäîìó ÷ëåíó îáû÷íîãî õèìè÷åñêîãî óðàâíåíèÿ â ýòîì ïðîãðàììèðîâàíèè ñîîòâåòñòâóþò äâà ïîëÿ - íàçâàíèå âåùåñòâà è ÷èñëåííûé êîýôôèöèåíò, ðàñïîëîæåííûå â îäíîé ãðóïïå è â îäíîé ñòðîêå. Åñëè â êà÷åñòâå íàçâàíèÿ èñïîëüçîâàòü õèì÷åñêóþ ôîðìóëó ñîåäèíåíèÿ, à êîýôôèöèåíòû ïîäáèðàòü, òî íàðóøåíèå ðàâåíñòâà óðàâíåíèÿ ðåçóëüòàòà ðàáîòû ïðîãðàììû - ìàññîâûõ ñîîòíîøåíèé - ê êàæäîé ïàðå óêàçàííûõ ïîëåé â ãëàâíîì îêíå äîáàâëåíî òðåòüå, ïîýòîìó êàæäàÿ ãðóïïà ïîëåé ñîäåðæèò òðè ñòîëáöà. Ââîä óðàâíåíèÿ ðåàêöèè çàêëþ÷àåòñÿ â âûáîðå íàçâàíèé ñîåäèíåíèé (êàê èñõîäíûõ âåùåñòâ, òàê è ïðîäóêòîâ ðåàêöèè), à åñëè âûêëþ÷åíà àâòîðàñïîçíàâàíèå êîýôôèöèåíòîâ óðàâíåíèÿ ðåàêöèè, òî è â çàïîëíåíèè ñîîòâåòñòâóþùèõ ïîëåé êîýôôèöèåíòîâ (ïðåìåùåíèå ìåæäó ïîëÿìè - ùåë÷êîì ìûøè íàä íóæíûì ïîëåì èëè êëàâèøàìè <Tab> èëè <Shift><Tab>, íàáîð ÷èñëîâûõ çíà÷åíèé - êëàâiøàìè öèôð íà êëàâèàòóðå,). Ðåäàêòèðîâàíèå ïîëÿ êîýôôèöèåíòà ïðèâîäèò ê âûêëþ÷åíèþ ýòîãî ïîëÿ èç ïðîöåññà àâòîðàñïîçíàâàíèÿ (âãî öâåò ìåíÿåòñÿ íà ãîëóáîâàòûé). Òàêîå áëîêèðîâàíèå (è íáðàòíàÿ ïîåðàöèÿ - ðàçáëîêèðîâàíèå) êîýôôèöèåíòà âîçìîæíî òàêæå ñ ïîìîùüþ ìåíþ, âûïîëíÿåìîãî ïðè íàæàòèè ïðàâîé êíîïêè ìûøè íàä ïîëåì êîýôôèöèåíòà. Ðàçáëîêèðîâàííîé ïîëþ âîçðàùàåòñÿ áåûé öâåò.

Ðàññìîòðèì ïðèìåð. Ïðè ââîäå óðàâíåíèÿ ðåàêöèè

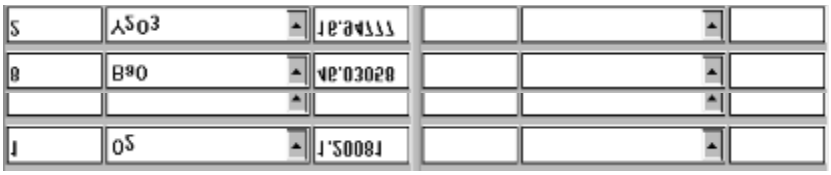
$$12CuO+8BaO+2Y_2O_3+O_2 = 4YBa_2Cu_3O_7$$

ïîëó÷àòñÿ òàêàÿ êàðòèíêà:



Åñëè óðàâíåíèå ââåäåíî ïðàâèëüíî è ïîëíîñòüþ, ñëåâà â íèæíåé ÷àñòè îêíà èíäèêàòîð ðåãèñòðèðóåò "Ìàòåðèàëüíûé áàëàíñ ÏÎÉÍÛÉ". Íåñîáëþäåíèå áàëàíñà ïî êàêîìó-ëèáî èç ýëåìåíòîâ îêðàøèâàåò ýòîò èíäèêàòîð â êðàñíûé öâåò ("...ÍÅ ÏÎÉÍÛÉ"). Â ýòîì ñëó÷àå ùåë÷îê ëåâîé êëàâiøåé ìûøè íà èíäèêàòîðå îòêðîåò äëÿ Âàñ îêíî áàëàíñà ïî ýëåìåíòàì. Åñëè àâòîðàñïîçíàâàíèå êîýôôèöèåíòîâ âêëþ÷åíà, òî âíèçó ñïðàâà èíäèêàòîð ðåãèñòðèðóåò ñîñòîÿíèå ðàñ÷åòà êîýôôèöèåíòîâ ("Ðåøåíèå âäèíñòâåííî" èëè "Ðåøåíèå ÍÅ âäèíñòâåííî" èëè "Ðåøåíèå îòñóòñòâóåò"). Â ñëó÷àå îòñóòñòâèÿ ðåøåíèÿ ùåë÷îê ëêâîé êëàâèøé ìûøè íàä íèäèêàòîðîì îòêðîåò äëÿ Âàñ îêíî ïðè÷èí îòñóòñòâèÿ ðåøåíèÿ.

Îáû÷íî óðàâíåíèå çàäàåò ëèøü ïðîïîðöèè ìåæäó ðåàãåíòàìè, äëÿ ðàñ÷åòà ðåàëüíûõ ìàññ ïðîãðàììå íóæíî óêàçàòü âåñ îäíîãî èç èñõîäíûõ âåùåñòâ èëè ïðîäóêòîâ ðåàêöèè, â çàâèñèìîñòè îò Âàøåé öåëè. Äëÿ ýòîãî çàíåñèòå çíà÷åíèå â ñîîòâåòñòâóþùåå ïîëå â êîëîíêàõ "Íà÷åñêè" èëè "Ìàññà". Îſëÿ ìàññ â ñòàëüíûõ ñòðî÷êàõ íàøåé òàáëöû òóò æå áóäóò ïðèâåäåíû â ñîîòâåòñòâèè ñ ïîñëåäíåé ââåäåííîé Âàìè öèôðîé. À ÷òîáû Âû íå çàáûâàëè, ÷òî ÿâëÿëîñü îòíîñèòåëüíî ÷èñëà ðàñ÷åòà, ïîñëåäíå îòðåäàêòèðîâàííîå ïîëå ìàññû áóäåò âûäåëåíî öâåòîì. Åñëè â ïðèâåäåííîì âûøå ïðèìåðå çàäàòü òðåáóåìóþ ìàññó ïðîäóêòà ðàâíóþ 100, òî êàðòèíêà áóäåò âûãëÿäåòü ïðèìåðíî òàê:



Ðåçóëüòàò ðàñ÷åòà ìîæíî îòìå÷àòàòü èëè ñêîïèðîâàòü â äðóãóþ ïðîãðàììó (ñðåäñòâàìè WINDOWS). Ââåäåíîå Âàìè óðàâíåíèå çàïîìèíàåòñÿ (ôàéë CONFIG.DB) è ïîýòîìó â êàæäûé íîâûé çàïóñê ïðîãðàììû Âû ìîæåòå ïðîäîëæàòü ðàáîòó ñ òîãî ìåñòà, íà êîòîðîì îñòàíîâèëèñü â ïðîøëûé ðàç.

ÂÍÈÌÀÍÈÅ! Ïðàâèëüíîñòü ðàñ÷åòà ïîðåäåëÿåòñÿ ñîäåðæèìûì áàçû äàííûõ î õèìè÷åñêèõ ñîåäèíåíèÿõ è áàçû äàííûõ î õèìè÷åñêèõ ýëåìåíòàõ, ïîñêîëüêó îíè èñïîëüçóþòñÿ ïðîãðàììîé äëÿ âû÷èñëåíèÿ ìîëÿðíûõ ìàññ.

×àñòî çàäàâàåìûå âîïðîñû
(ïî ïðåäûäóùèì âåðñèÿì ïðîãðàììû)

Âîïðîñ: *Ïî÷åìó ïîñëå âûáîðà èñõîäíûõ ðåàãåíòîâ ïðîãðàììà íå çàïëéíÿåò ïîëÿ ïðîäóêòîâ ðåàêöèè ñàìîñòîÿòåëüíî?*
Îòâåò: Îíà íå äëÿ ýòîãî ïðåäíàçíà÷åíà. Âûáðèòå ïðîäóêòû ðåàêöèè - è ïðîãðàììà ðàññ÷èòàåò êîýôôèöèåíòû óðàâíåíèÿ ðåàêöèè. Çàäàéòå ìàññó ïîñëåäíåãî èç ðåàãåíòîâ - è îíà ïîäñ÷èòàåò ìàññû îñòàëüíûõ. Íî íå çàäàâàéòå åé âîïðîñîâ î ñìûñëå æèçíè - äëÿ èõ ðåøåíèÿ ó íåå íåäîñòàòî÷íî äàííûõ.

Âîïðîñ: *Ïî÷åìó âìåñòî çàãîëîâêîâ êîëîíîê â ãëàâíîì îêíå è âìåñòî òàáëöû â ðàñ÷åòå èäåò êàêàÿ-òî àáðàêàäàáðà?*
Îòâåò: Äëÿ âûâîäà óêàçàííûõ òåêñòîâ ïðîãðàììà ïûòàåòñÿ èñïîëüçîâàòü øðèôòû, óêàçàííûå â ïåðåìåííûõ GraphicFontName= è PrintFontName= ini-ôàéëà urchmclc.ini. Îí-âèäèìîìó, â Âàøåì âàðèàíòå óñòàíîâêè óêàçàíû øðèôòû, íå èìåþùèå ñèìâîëîâ êèðèëëèöû. Ïîïðîáóéòå âûáðàòü øðèôò â îêíå ïå÷àòè (ïóíêò ìåíþ **Ôîðìà\Øðèôò**). Ïðîáëåìû ñ øðèôòîì îêíà WINDOWS HELP ó Âàñ, ïî-âèäèìîìó, ðåøåíû, ðàç óæ Âû ñìîãëè âñå ýòî ïðî÷åñòü. ßðëû÷êè ïîäñêàçîê, ïóíêòû ìåíþ è áîëüøèíñòâî íàäïèñåé â îêíàõ ïðîãðàììû âûïîëíåíû íà ñèñòåìíûõ øðèôòàõ WINDOWS, ïîýòîì ñ íèì ó Âàñ çàòðóäíåíèé áûòü íå äîëæíî, åñëè ðóñèôèêàöèÿ Âàøåé âåðñèè WINDOWS âûïîëíåíà êîððåêòíî.

Âîïðîñ: *Ïî÷åìó âî âðåìÿ ðåäàêòèðîâàíèÿ ÷èñëîâûõ ïîëåé ïðîãðàììà òî è äåëî çàÿâëÿåò ìíå îøèáêó ëëè ïðîñòî äàåò çâóêîâîé ñèãíàë âìåñòî ââîäà çàïÿòîé?*
Îòâåò: Îñâåæèòå âåðñèþ ïðîãðàììû - íà÷èíàÿ ñ 1.2, "Õèì÷åñêèé êàëüêóëÿòîð" íå òàê ïðèâåðæåíà ê äåñÿòè÷íîìó ðàçäåëèòåëþ. Äëÿ ïîëüçîâàòåëåé âåðñèè 1.1 è íèæå - ñëåäóþùèé ñîâåò: íå ïóòàéòå äåñÿòè÷íóþ òî÷êó ñ çàïÿòîé. Ïåðâàÿ äîïóñòèìà (à ÷àñòî è íåîáõîäèìà) ïðè ââîäå ÷èñëè, à âòîðàÿ - íåò. Ðàçáåðèòåñü ñ íàñòðîéêîé Âàøåé êëàâèàòóðû è èñïîëüçóéòå òî÷êó äëÿ ÷èñëîâûõ çíà÷åíèé, à çàïÿòóþ - äëÿ òåêñòîâûõ.

Âîïðîñ: *Ïî÷åìó âî âðåìÿ ðåäàêòèðîâàíèÿ íàçâàíèÿ õèì÷åñêîãî ñîåäèíåíèÿ îíî âûãëÿäèò èíà÷å, ÷åì â èíûå ìîìåíòû âûïîëíåíèÿ ïðîãðàììû?*
Îòâåò: Íàçâàíèå õèì÷åñêîãî ñîåäèíåíèÿ õðàíèòñÿ â ÁÄ â âèäå îáû÷íîé ñòðîêè áåç ïîäñòðî÷íèêîâ è çàìåí ñèâîëîâ, ïîýòîìó ÁÄ î õèì÷åñêèõ ñîåäèíåíèÿõ ìîæåò áûòü ëåãêî èñïîëüçîâàíà â äðóãèõ Âàøèõ ïðèëîæåíèÿõ. Îäíàêî ïðîãðàììà "Õèì÷åñêèé êàëüêóëÿòîð" äëÿ óäîáñòâà âîñïðèÿòèÿ ïîëüçîâàòåëåì õèì÷åñêèõ ôîðìóë ïîñëå èõ ïîñòðîí÷íèêîâ è çàìåí ýëåìåíòîâ (íå òðîãàÿ êîýôôèöèåíòû, ñòîÿùèå ïåðåä ãðóïïàìè â ñîåäèíåíèÿõ òèïà êðèñòàëëîãèäðàòà), çàìåíÿåò ñèìâîë ìàòåìàòè÷åñêîãî óìíîæåíèÿ <*> íà áîëåå ïðèâû÷íûé â õèì÷åñêîì ôîðìóëàõ ñèìâîë <·> è ò.ï.. Íî äëÿ Âàñ îñòàâëåíà âîçìîæíîñòü óâèäåòü è îöåíèòü òîò âèä íàçâàíèÿ, â êàêîì îíî õðàíèòñÿ â ÁÄ. Yòî ìîæíî ñäåëàòü â ìîìåíò ðåäàêòèðîâàíèÿ íàçâàíèÿ â îêíå ÁÄ î õèì÷åñêîõ ñîåäèíåíèÿõ. Åñëè æå Âû ââîäèòå íîâóþ çàïèñü ÁÄ ÷åðåç âûáîð ïóíêòà "Íîâîå ñîåäèíåíèå" â âûïàäàþùåì ñïèñêå ïîëÿ íàçâàíèÿ â ãëàâíîì îêíå, òî ó Âàñ åñòü âîçìîæíîñòü óâèäåòü îáà ïðåäñòàâëåíèÿ íàçâàíèÿ îäíîâðåìåííî.

Âîïðîñ: *Ó ìåíÿ çíàêîìîãî ïðîãðàììà "Õèì÷åñêèé êàëüêóëÿòîð" óñòàíîâëåíà äîâîëüíî äàâíî è ïîñòîÿííî "ïàðîñëà" îáøèðíîé áàçîé äàííûõ î õèì÷åñêèõ ñîåäèíåíèÿõ. Íåëüçÿ ëè ïåðåíåñòè åãî ÁÄ íà ìîé êîìïüþòåð ê íåäàâíî óñòàíîâëåííîì ýêçåìïëÿðó ïðîãðàììû?*
Îòâåò: Â ñîîòâåòñòâèè ñ äåéſòâóþùèì (1997ã.) â Ðîññèè çàêîíîäàòåëüſòâî ïðàâèò íà ÁÄ îáëàäàåò åå ñîçäàòåëü (Âàø çíàêîìûé), åñëè íå ñóùåſòâóåò äîãîâîðà î ïåðåäà÷å èì ïðàâ íà íåå äðóãèì ëèöàì. Òàê ÷òî ïðåæäå âñåãî íåîáõîäèìî åãî ñîãëàſåíèå. À òåõíè÷åſêè ïðîãëåìà ìîæåò áûòü ðåøåíà ââóìÿ ïóòÿìè:
1) çàìåíà Âàøèõ ôàéëîâ **OUR .*** â êàòàëîãå (ïàïêå) ïðîãðàììû "Õèì÷åſêèé êàëüêóëÿòîð" íà àíàëîãè÷íûå ſ êîìïüþòåðà Âàøåſî çíàêîìîſî - íî â ýòî ſëó÷àå ïðîïàäóò òå äàííûå, êîòîðûå õðàíèëèſü â Âàøåé ÁÄ;
2) ſëèÿíèå áàç äàííûõ ìîæåò áûòü âûſïëíåſî ſðåäſòàâèì òåõ ſèſòåì óïðàâëåſèÿ áàçàìè

äàííûõ, êîòîðûå ïîääåðæèâàþò Paradox (íàïðèìåð, Borland DataBase DeskTop). Åñëè Âû íå ïîíÿëè, î ÷åì ðå÷ü, òî Âàì íåîáõîäèìà ïîìîùü ñïåöèàëèñòà.
Êîììåíòàðèé: Åñëè ó Âàñ íåò çíàêîìîãî ñ áîëåå-ìåíåå ïîëíîé ÁÄ ïî Âàøåé òåìàòèêå, îáðàòèòåñü ê àâòîðó ïðîãðàììû - âîçìîæíî, ó íåãî íàéäåòñÿ ÷òî-íèáóäü äëÿ Âàñ. Íî ðàçäóâàòü ñâîè ÁÄ åñëè ïîëüçîâàòåëüñêèõ - â äëèííûõ ñïèñêàõ Âàì ïðèäåòñÿ äîëüøå êîïàòüñÿ, äà è ðàáîòà ïðîãðàììû ìîæåò çàìåäëèòüñÿ, åñëè Âàø êîìïüþòåð íå îáëàäàåò áîëüøîé ïðîèçâîäèòåëüíîñòüþ (íàïðèìåð, 386SX).

Âîïðîñ: *Â íåêîòîðûõ ìèõ ðåàêòèâàõ ñîäåðæàòñÿ ïðèìåñè, íå âëèÿþùèå íà õîä ðåàêöèè, îí íà êîòîðûå ÿ âûíóæäåí ïîñòîÿííî ðàñ÷èùàòü ïîðâêè ïðè âçâåøèâàíèè. Íåëüçÿ ëè çàòàêîâ ïðîãðàììó ýòî äåëàòü çà ìåíÿ?*
Îòâåò: Ââåäèòå â çàïèñü ÁÄ î òàêèõ õèì÷åñêèõ ñîåäèíåíèÿõ ñâåäåíèÿ î ñîäåðæàùèõñÿ â íèõ ïðèìåñÿõ. Íàïðèìåð, La2O3 ñ 11.05âåñ.% H2O ìîæåò áûòü çàïèñàí êàê La2O3 ·2.247 H2O :

Ìîëÿðíàÿ ìàññà òàêîãî âåùåñòâà áóäåò ðàññ÷èòàíà ïðîãðàììîé ñ ó÷åòîì âõîäÿùåé â ñîñòàâ âîäû è, ñîîòâåòñòâåííî, íàâåñêà áóäåò ïîðåäëåíà òàêæå ñ ó÷åòîì ýòîé ïîïðàâêè. Îäíàêî åñëè âû õîòèòå ïîëüçîâàòüñÿ [àâòîðàññòàíîâêîé êîýôôèöèåíòîâ](), òî íå çàáóäüòå âêëþ÷èòü ïðèçíàê (â ïðèâåäåííîì ïðèìåðå - âîäó) â íàáîð ïðîäóêòîâ ðåàêöèè - äàæå åñëè îíà âñåãî ëèøü èñïàðÿåòñÿ ïðè ñèíòåçå.

Åùå ëó÷øå ïðè çàïîëíåíèè çàïèñè î òàêîì ñîåäèíåíèè âîñïîëüçîâàòüñÿ [ìàñòåðîì ðàñòâîðîâ](). Íî íåðåñ÷èòàííûå ðåçóëüòàòû ïðèìåñè â ìîëüíûå äîëè, èñïîëüçóåìûå â çàïèñè ÁÄ, è ïðè ýòîì íåâûïîëíåíèè òî÷íîñòè. Ïîñêîëüêó â êà÷åñòâå êàê ðàñòâîðèòåëÿ, òàê è ðàñòâîðåííîãî âåùåñòâà ìîæåò áûòü ïîäîãíàëåíî ëþáîå ñîåäèíåíèå, ýòî ñîîòíîøåíèå íå òî÷íîé äëÿ ñîáñòâåííî ðàñòâîðà, íî è äëÿ ëþáûõ áèíàðíûõ ñìåñåé.

Âîïðîñ: *Ìíå ÷àñòî ïðèõîäèòñÿ ãîòîâèòü ñìåñè (ñïëàâû, ðàñòâîðû) ñ çàäàííûì ïðîöåíòíûì ìåæäó ñîñòàâëÿþùèìè. Ìîæåò ëè ïðîãðàììà ïîìî÷ü â ïîäáîðó ðàñ÷åòîâ?*
Îòâåò: Äà, êîíå÷íî. Ïðîãðàììà íè÷åãî íå çíàåò î õèì÷åñêèõ ñâÿçÿõ, î òåðìîäèíàìèêå è ò.ï.. Äëÿ íåå õèì÷åñêîå ñîåäèíåíèå íè÷åì íå îòëè÷àåòñÿ îò ñìåñè ýëåìåíòîâ ñ òêêñêðîâàííûì ïðîöåññîì. Îäíàêî íà ïóòàéòå ì îëüíûå è âåñîâûå ïðîöåíòû ïðè ââîäå çàïèñåé î Âàøèõ ñìåñÿõ (ñì. âûøå ïðèìåð ñ La2O3) è èñïîëüçóéòå [ìàñøòàá ðàñòâîðà](). Åùå áîëåå ïðîñòî ñîîòíîøåíèÿ. Òîãäà Âû ìîæåòå, íå çàìåíÿÿ ñìåñü â ÁÄ, ñîñòàâèòü åå èç êîìïîíåíòîâ ïðÿìî â ãëàâíîì îêíå, [òêêñèðóÿ êîýôôèöèåíòû]() ïðè íèõ.

Âîïðîñ: *Ïî÷åìó ïðîãðàììà íå äàåò íàçâàíèÿ ñîåäèíåíèÿì àâòîìàòè÷åñêè ïîñëå çàìåíåíèÿ ïëåé ýëåìåíòîâ è êîýôôèöèåíòîâ? Ïî÷åìó äëÿ ýòîãî ïðèõîäèòñÿ äîïîëíèòåëüíî íàæèìàòü êíîïêó?*
Îòâåò: Äåëî â òîì, ÷òî ïðîãðàììà ÷àñòî íå â ñîñòîÿíèè îäíîçíà÷íî âûäåëèòü ãðóïïû, ïîäëåæàùèå íáúåäèíåíèþ â ôîðìóëàõ (íàïðèìåð, Ca(OH)2 èëè CaO·H2O) è ïîýòîìó ñîñòàâëÿåò íàçâàíèÿ áåç ïðåãðóïïèðîâîê (íàïðèìåð, CaO2H2). Îäíàêî ìíîãèå ïðåäïî÷èòàþò èìåòü äåëî ñ íàçâàíèÿìè â ïðèâû÷íîì âèäå è çàôiòyò âíåñòè â ôîðìóëó ïîïðàâêè ïî ñâîåìó âêóñó, âïëîòü äî ïîñòðîåíèÿ òåêſòîâ òèïà "Äèäðîêñèä êàëüöèÿ" èëè "Ãàøåíèå êàëüöèÿ". Èìåíî äëÿ íèõ ñâÿçü ìåæäó ýëåìåíòíûì ñîñòàâîì è íàçâàíèåì ñîåäèíåíèÿ ñäåëàíà íå æåñòêîé, ñ âîçìîæíîñòüþ ðåäàêòèðîâàíèÿ. Íî è äëÿ òåõ, êòî äîâåðÿåò ñîñòàâëåíèå íàçâàíèÿ ïðîãðàììå, íå îáÿçàòåëüíî íàæèìàòü íà êíîïêó  . Åñëè íàçâàíèå îñòàëîñü ïóñòûì ïðè âûõîäå èç îêíà ðåäàêòèðîâàíèÿ èëè ïðè ïåðåõîäå ê ðåäàêòèðîâàíèþ äðóãîé çàïèñè, ïðîãðàììà ñäåëàåò íàçâàíèå èç ñîñòàâà ñàìà, êàê åñëè áû Âû íàæàëè íà ýòó êíîïêó.

Âîïðîñ: *Ïî÷åìó ïðîãðàììà íå òîëüêî íå ìîæåò ðàññòàâèòü êîýôôèöèåíòû ðåàêöèè òàêîé-òî, íî è*

íåïðàâèëüíî ðàñ÷èòûâàåò íàâåñêè äëÿ íåå ïîñëå ðàñòàíîâêè êîýôôèöèåíòîâ âðó÷íóþ?
Îòâåò: Òèïè÷íàÿ ïðè÷èíà - íåâåðíûå çàïèñè ÁÄ î õèì÷åñêèõ ñîåäèíåíèÿõ, îòíîñÿùèåñÿ ê èñõîäíûì âåùåñòâàì è ïðîäóêòàì ðàñïàäêàåìîé ðåàêöèè. Îí êðàéíå ìåðå îäíà èç ýòèõ çàïèñåé áûëà ââåäåíà ñ îøèáêàìè - èñïðàâüòå èõ. Â äåëå ëîêàëèçàöèè îøèáîê Âàì òàêæå îãóò ïîìî÷ü îêîí áàëàíñà ïî ýëåìåíòàì è îêîí ïðè÷èí îòóòñòâèÿ ðåøåíèÿ. Â ãèïîòåòè÷åñêîì ñëó÷àå íåâåðíîé ðàáîòû ïðîãðàììû ïðè îòñóòñòâèè îøèáîê â ÁÄ ñâÿæèòåñü ñ ðàçðàáîò÷èêîì.

Âîïðîñ: *Êàêèå èçìåíåíèÿ ïëàíèðóåòñÿ îñóùåñòâèòü â ñëåäóþùåé âåðñèè ïðîãðàììû?*
Îòâåò: Âñå çàðåãèñòðèðîâàííûå ïîëüçîâàòåëè ìîãóò îòïðàâèòü ñâîè ïîæåëàíèÿ ïî E-mail àâòîðà (aal@ihim.ural.ru èëè lakhtin@hotmail.com). Íåâîçìîæíî îáåùàòü, ÷òî âñå ïîè áóäóò ðåàëèçîâàíû, íî ìîæíî ãàðàíòèðîâàòü, ÷òî âñå îíè áóäóò ðàñ÷èòðåíû.

Âîïðîñ: *Ïî÷åìó àâòîð íå îòâå÷àåò íà ìîè âîïðîñû ïî ýëåêòðîííîé ïî÷òå?*
Îòâåò: Âû íå çàðåãèñòðèðîâàëè ñâîþ êîïèþ ïðîãðàììû.

Îêíî áàëàíñà ïî ýëåìåíòàì

English

Ýòî îêíî ïîÿâëÿåòñÿ ïðè ùåë÷êå ëåâîé êëàâèøåé ìûøè íà èíäèêàòîðå ìàòåðèàëüíîãî áàëàíñà â ãëàâíîì îêíå â ñëó÷àå íåïîëíîãî áàëàíñà. Îêíî ñîäåðæèò èíôîðìàöèþ î ïîýëåìåíòíîì áàëàíñå. Â âåðõíåé ÷àñòè îêíà êðàñíûì öâåòîì âûäåëåíû ýëåìåíòû, ïî êîòîðûì óðàâíåíèå ðåàêöèè ïðè çàäàííûõ êîýôôèöèåíòàõ íå ÿâëÿåòñÿ ñáàëàíñèðîâàííûì. Â ñðåäíåé ÷àñòè ðåãóëÿðíûì öâåòîì èçîáðàæåíû ýëåìåíòû, áàëàíñ ïî êîòîðûì âûïîëíÿåòñÿ. Â íèæíåé ÷àñòè ðàñïîëîæåíû êíîïêè:

Ok - çàêðûòèå îêíà áàëàíñà, âîçâðàùåíèå â ãëàâíîå îêíî;

Help - âûçîâ îêíà ñïðàâêè.

Îêíî òàêæå îáëàäàåò íåêîòîðûìè ñòàíäàðòíûìè ýëåìåíòàìè èíòåðôåéñà WINDOWS: çàãîëîâêîì, êíîïêîé ñèñòåìíîãî ìåíþ è ÿâëÿåòñÿ ïåðåìåùàåìûì.

Îêíî áàëàíñà ìîæåò îêàçàòüñÿ ïîëçíûì äëÿ òåõ, êòî õî÷åò äîáèòüñÿ ïîëíîãî áàëàíñà ïðè ðàññòàíîâêå êíýôôèöèåíòîâ óðàâíåíèÿ ðåàêöèè âðó÷íóþ. Îäíàêî åñëè ýòà öåëü âîîáùå äîñòèæèìà ïðè äàííîì íàáîðå ðåàãåíòîâ, òî äîñòàòî÷íî âêëþ÷èòü àâòîðàññòàíîâêó êîýôôèöèåíòîâ , îñâîáîäèòü çàáëîêèðîâàííûå êíýôôèöèåíòû- è ðåøåíèå áóäåò íàéäåíî ïðîãðàììíé. Äðóãîå äåëî, åñëè íàéäåííûå ðåøåíèå íå ÿâëÿåòñÿ åäèíñòâåííûì - òîãäà âûáîð ïðèäåòñÿ äåëàòü ïîëüçîâàòåëþ è îêíî áàëàíñà ïî ýëåìåíòàì ïîìîæåò ðàñøèôðîâàòü âîçìîæíûå îøèáêè. Åùå áîëüøóþ ïîìîùü ýòî îêíî ìîæåò îêàçàòü òåì, êòî íå õî÷åò ñîñòàâëÿòü ïëîñêóþ óðàâíåíèå ðåàêöèè, ÷àñòü ðåàãåíòîâ â êîòîðîé ïîÿâëÿåòñÿ (èëè âûäåëÿåòñÿ) â íóæíûõ ïðîïîðöèÿõ ñàìîñòîÿòåëüíî (èç àòîìñôåðû, ðàñòâîðèòåëÿ è ò.ï.).

Îêíî ïðè÷èí îòñóòñòâèÿ ðåøåíèÿ

English

Ýòî îêíî ïîÿâëÿåòñÿ ïðè ùåë÷êå ëåâîé êëàâèøåé ìûøè íà èíäèêàòîðå ñîðàâà â íèæíåé ÷àñòè ãëàâíîãî îêíà â ñëó÷àå îòñóòñòâèÿ ðåøåíèÿ. Îêíî ñîäåðæèò èíôîðìàöèþ î âîçìîæíûõ ïðè÷èíàõ îòñóòñòâèÿ ðåøåíèÿ. Â íèæíåé ÷àñòè îêíà ðàñïîëîæåíû êíîïêè:

Ok - çàêðûòü îêíà, âîçâðàùåíèå â ãëàâíîå îêíî;

Help - âûçîâ îêíà ñïðàâêè.

Îêíî òàêæå îáëàäàåò íåêîòîðûìè ñòàíäàðòíûìè ýëåìåíòàìè èíòåðôåéñà WINDOWS: çàãîëîâêîì, êíîïêîé ñèñòåìíîãî ìåíþ è ÿâëÿåòñÿ ïåðåìåùàåìûì.

Àíàëèç ïðè÷èí îòñóòñòâèÿ ðåøåíèÿ ïðè âêëþ÷åíîé àâòîðàññòàíîâêå êîýôôèöèåíòîâ ðåàëèçîâàí â ïðîãðàììå â ìèíèìàëüíîì îáúåìå. Åñëè Âàì íåîáõîäèì áîëåå ïîäðîáíûé àíàëèç, ñâÿæèòåñü ñ ðàçðàáîò÷èêîì ïðîãðàììû è ïîëó÷èòå Âàø êóã çàäà÷. Âîçìîæíî, Âàøà àðãóìåíòàöèÿ îêàæåòñÿ äîñòàòî÷íî óáåäèòåëüíîé äëÿ ðàçâèòèÿ ýòîãî íàïðàâëåíèÿ â ñëåäóþùåé âåðñèè ïðîãðàììû.

Ìàñòåð ðàñòàíîâêà

English

Íàçíà÷åíèå - ïîìîùü â çàïîëíåíèè çàïèñåé ÁÄ î õèìè÷åñêèõ ñîåäèíåíèÿõ, îòíîñÿùèõñÿ ê áèíàðíûì ñìåñÿì (æèäêèì è òâåðäûì ðàñòâîðàì, âåùåñòâàì ñ ïðèìåñÿìè è ò.ï.). Îñóùåñòâëÿåò ïåðåíîñ ðàçëè÷íûõ ïðåäñòàâëåíèé êîíöåíòðàöèè â ìîëüíûå äîëè, ïðåíîñèìûå íåïîñðåäñòâåííî â çàïèñü ÁÄ.

Âûçîâ ìàñòåðà îñóùåñòâëÿåòñÿ ïðè íàæàòèè êíîïêè  â îêíå ðåäàêòèðîâàíèÿ ÁÄ î õèìè÷åñêèõ ñîåäèíåíèÿõ. Áóäüòå âíèìàòåëüíû - ìàñòåð çàïîëíÿåò **òåêóùþ çàïèñü ÁÄ**! Åñëè ðàñòâîð äîëæåí áûòü çàïèñàí â äîïîëíåíèå ê óæå ñóùåñòâóþùèì çàïèñÿì, ïðåä âûçîâîì ìàñòåðà íå çàáóäüòå íàæàòü êíîïêó **Âñòàâêà**. Åñëè äîñòóï ê ÁÄ îïëó÷åí ïóòåì âûáîðà ñëóæåáíîé ôðàçû "Íîâîå ñîåäèíåíèå" â âûïàäàþùåì ñïèñêå ëþáîãî ïîëÿ íàçâàíèÿ â ãëàâíîì îêíå, òî Âû óæå èìåòå äåëî ñ íîâîé çàïèñüþ.

Â âåðõíåé ÷àñòè îêíà ìàñòåðà ðàñòâîðîâ ïðèñóòñòâóþ äâà ïîëÿ *Âåùåñòâî* è *Ðàñòâîðèòåëü*, ñîäåðæèìîå êîòîðûõ Âû ìîæåòå âûáðàòü èç âûïàäàþùèõ ñïèñêîâ, ïðåäñòàâëÿþùèõ íàçâàíèÿ ñîäåðæàùèõñÿ â ÁÄ ñîåäèíåíèé. Íèæå ðàñïîëîæåíî ïîëå, âûïàäàþùèé ñïèñîê êòòîðîâ ñîäåðæèò ðàçëè÷íûå ñîîáùåíèÿ êîíöåíòðàöèè (çäåñü âåçäå èìåòñÿ â âèäó êîíöåíòðàöèÿ âåùåñòâà â ðàñòâîðèòåëå, à íå íàîáîðîò). Ñîäåðæèìîå ýòîãî ïîëÿ ïîðåäåëÿåò ÷èñëî è íàçíà÷åíèå ÷èñëîâûõ ïîëåé ïîä íèì, çàïîëíåíèå êîòîðûõ íåîáõîäèìî äëÿ ïðåâîä êîíöåíòðàöèè â ìîëüíûå äîëè. Íà äàííûé ìîìåíò ñîîáùåíèà ñîîòíîøåíèÿ â ñìåñè. Ñóìì ìîëüíûõ äîëåé âåùåñòâà è ðàñòâîðèòåëÿ ðàâíà åäèíèöå);
2) Ìàññîâàÿ äîëÿ (õàðàêòåðèçóåò ìîëÿðíûå ñîîòíîøåíèÿ â ñìåñè. Ñóìì ìàññîâûõ äîëåé âåùåñòâà è ðàñòâîðèòåëÿ ðàâíà åäèíèöå);
3) Ìîëÿëüíîñòü (÷èñëî ìîëåé âåùåñòâà íà îäèí êèëîãðàìì ðàñòâîðèòåëÿ);
4) Ìîëÿðíîñòü (÷èñëî ìîëåé âåùåñòâà â îäíîì ëèòðå ðàñòâîðà - äëÿ ïðåñ÷åòà òðåáóåìîñòè ïîíîñòü ðàñòâîðà);
5) Íîðìàëüíîñòü (÷èñëî ãðàìì-ýêâèâàëåíòîâ âåùåñòâà â îäíîì ëèòðå ðàñòâîðà - êðîìå ïîíîñòè ðàñòâîðà, íóæíî óêàçàòü êîëè÷åñòâî ãðàìì-ýêâèâàëåíòîâ â îäíîì ìîëå âåùåñòâà).

Â íèæíåé ÷àñòè îêíà ðàñïîëîæåíû ñëåäóþùèå êíîïêè óïðàâëåíèÿ:
Ok - Âûõîä èç ìàñòåðà ðàñòâîðîâ ñ çàíåñåíèåì ïîëó÷åííûé ñìåñè â òó çàïèñü ÁÄ î õèìè÷åñêèõ ñîåäèíåíèÿõ, â ïðîöåññå ðåäàêòèðîâàíèÿ êîòîðîé íî áûë âûçâàí. Ïðè ýòîì ïðîãðàììà ïðîèçâîäèò ïðîâåðêó íà äîïóñòèìîñòü çíà÷åíèé â ïîëÿõ îêíà ìàñòåðà, ïåðåñ÷èò êîíöåíòðàöèè è çàïîëíåíèå ïîëåé ýëåìåíòîâ è êîýôôèöèåíòîâ ýòîé çàïèñè ÁÄ (ïðîãðàììà âî èçáåæàíèå ïîÿâëåíèÿ ñëèøêîì áîëüøèõ ÷èñåë â ïîëÿõ êîýôôèöèåíòîâ èíîãäà äëèò èõ íà 10 (èëè íà 100, 1000 è ò.ä.)).
Cancel - Âûõîä èç ìàñòåðà áåç èçìåíåíèÿ òåêóùåé çàïèñè ÁÄ.
Help - Âûçîâ äàííîãî îêíà ñïðàâêè.
Îêî òàêæå îáëàäàåò íåêîòîðûìè ñòàíäàðòíûìè ýëåìåíòàìè èíòåðôåéñà WINDOWS: çàãîëîâêîì, êíîïêîé ñèñòåìíîãî ìåíþ è ÿðëûêàõ ïðåìåùàåìûì.

Ìàñòåð ðàñòâîðîâ - ðåêîìåíäóåìûé ïóòü çàíåñåíèÿ â ÁÄ çàïèñåé î ðàñòâîðàõ (ñìåñÿõ), êîíöåíòðàöèÿ êîòîðûõ âûðàæåíà íå â ìîëüíûõ äîëÿõ. Òî÷íîñòü ïðèçâîäèìîãî ìàñòåðîì ïðåðñ÷èòà ïî âûáðàííûì çíà÷åíèÿì â ïîëÿ êîýôôèöèåíòîâ ìîëüíûõ ñîîòíîøåíèé, ðàññ÷èòàííûõ èç êîíöåíòðàöèè äðóãèõ ñðåäñòâàìè, èái ðàçìåð ïîëé ââîäà îãðàíè÷åí ñóùåñòâîâíî ñèëüíåå, ÷åì âíóòðåííÿÿ ðàçðÿäíîñòü ÷èñëà ñ ïëàâàþùåé òî÷êîé. Îáíâêî äàæå ýòîé òî÷íîñòè Âàì ìîæåò íå õâàòèòü, åñëè Âû íàìåðåíû âíîñèòü â ÁÄ ñëèøêîì ðàçáàëëíûå ðàñòâîðû. Â òàêîì ñëó÷àå ñâÿæèòåñü ñ ðàçðàáîò÷èêîì ïðîãðàììû.

Åñëè Âàñ íå óâîëåòâîðÿåò ôîðìóëà, ïîëó÷åííàÿ ñ ïîìùüþ ìàñòåðà ðàñòâîðîâ, ïîðîáóéòå âîñïîëüçîâàòüñÿ ñðåäñòâîì äëåíèÿ âñåõ êîýôôèöèåíòîâ íà îäíî ÷èñëî (ïóòåì äâîéíîãî ùåë÷êà ëåâîé êíîïêè ìûøè íàä ïîëåì êîýôôèöèåíòà â çàïèñè ñîåäèíåíèÿ). Ýòî ïóòü ïðèâåäåíèÿ ôîðìóëû íå ñíèæàåò òî÷íîñòè êîýôôèöèåíòîâ â îòëè÷èå îò ðåäàêòèðîâàíèÿ âðó÷íóþ.

Ðåãèñòðàöèÿ

English

Ïðîãðàììà Õèìè÷åñêèé êàëüêóëÿòîð íå ÿâëÿåòñÿ áåñïëàòíîé. Îíà ðàñïðîñòðàíÿåòñÿ êàê SHAREWARE, òî åñòü åñëè Âû íàìåðåíû èñïîëüçîâàòü ýòó ïðîãðàììó, òî Âàì íåîáõîäèìî çàðåãèñòðèðîâàòüñÿ â êà÷åñòâå ïîëüçîâàòåëÿ. Äëÿ ýòîãî Âû äîëæíû çàïîëíèòü ðåãèñòðàöèîííóþ îôîðìó è ïîñëàòü åå ðàçðàáîò÷èêó ïî ýëåêòðîííîé ïî÷òå **lakhtin@hotmail.com**

Åñëè Âû õîòèòå çàðåãèñòðèðîâàòü íåñêîëüêî êîïèé (à ýòî íåîáõîäèìî äëÿ óñòàíîâêè ïðîãðàììû íà íåñêîëüêèõ êîìïüþòåðàõ, à òàêæå â ñåòè), íóæíî óêàçàòü òðåáóåìîå êîëè÷åñòâî - ïðåäóñìîòðåíû ñóùåñòâåííûå ñêèäêè. Åñëè Âàì íå ïîäõîäèò ñòàíäàðòíûé ñïîñîá âíåñåíèÿ ðåãèñòðàöèîííîãî âçíîñà (ïî÷òîâûé ïåðåâîä ñóììû, ýêâèâàëåíòíî $30), óêàæèòå ïðåäïî÷òèòåëüíûå äëÿ Âàñ ñïîñîáû. Â îòâåòíîì ïiñüìå Âàì áóäóò ñîîáùåíû ðåêâèçèòû äëÿ ïåðå÷èñëåíèÿ âçíîñà, åãî òî÷íàÿ ñóììà íà ýòîò ìîìåíò, à òàêæå èíôîðìàöèÿ î ïîñëåäíåé âåðñèè ïðîãðàììû. Ïîñëå ïîëó÷åíèÿ ðàçðàáîò÷èêîì ðåãèñòðàöèîííîãî âçíîñà Âàì áóäåò âûñëàí ïðèâàòíûé Âàøåé êîïèè ïðîãðàììû ðåãèñòðàöèîííûé íîìåð, ñ èíñòðóêöèåé ïî åãî ïðèìåíåíèþ, à äëÿ ñåòåâîãî âàðèàíòà è èíñòðóêöèÿ ïî óñòàíîâêå â ñåòè. Ïîñëå âûïîëíåíèÿ èíñòðóêöèè ñâîé ðåãèñòðàöèîííûé íîìåð Âû âñåãäà ñìîæåòå íàéòè â îêíå êðàòêîé èíôîðìàöèè î ïðîãðàììå (ïóíêò ìåíþ Ñïðàâêà/Î_ïðîãðàììå â ãëàâíîì îêíå). Ïðîãðàììà ïðèíàäëåæèò âûâîäà ðåçóëüòàòîâ íà ïðèíòåð è â Áóôåð Îáìåíà WINDOWS. Çàïàíî Âû èçáàâèòåñü îò ëèöåíçèîííîé çàñòàâêè ñâåðõ íåîáõîäèìîãî äëÿ ðàáîòû ïðîãðàììû âðåìåíè.

Çàðåãèñòðèðîâàííûå ïîëüçîâàòåëè èìåþ ïðàâî:

- ïîëó÷àòü ïî ýëåêòðîííîé ïî÷òå îòâåòû íà ñâîè âîïðîñû è ïðåäëîæåíèÿ ïî ïîâîäó ïðîãðàììû, ñîïðîâîæäàåìûå íîìåðîì è ÔÈÎ,
- ïîëó÷àòü èíôîðìàöèþ î íîâûõ âåðñèÿõ ïðîãðàììû è ñêèäêè ïðè èõ ïîêóïêå.

Íåçàðåãèñòðèðîâàííóþ âåðñèþ ïðîãðàììû ìîæíî ñâîáîäíî, ïðåäíîñèòü íà äóãèå êîìïüþòåðû è èñïîëüçîâàòü â òå÷åíèå îäíîãî ìåñÿöà. Äàëüíåéøåå èñïîëüçîâàíèå áåç ðåãèñòðàöèè, à òàêæå èçìåíåíèå îòäåëüíûõ ÷àñòåé ïðîãðàììû èëè åå êîìïèëêôîíñòè, ÿâëÿåòñÿ íàðóøåíèåì àâòîðñêèõ ïðàâ ðàçðàáîò÷èêà è, ñîîòâåòñòâåííî, äåéſòâóþùåãî çàêîíîäàòåëüſòâà.

Ðàñſìàòðèâàþſòñÿ ïðåäëîæåíèÿ î ðàçìåùåíèè â ñëåäóþùåé âåðſèè ïðîãðàììû ðåêëàìſûõ âſòàâîê.

Îñíîâíûå ïðåèìóùåñòâà SHAREWARE ïåðåä SOFTWARE äëÿ êîíå÷íîãî ïîëüçîâàòåëÿ, êàê ýòî âèäèòñÿ àâòîðó

Ïîëüçîâàòåëü íå ïîêóïàåò êîòà â ìåøêå - îí èìååò âîçìîæíîñòü óáåäèòüñÿ, ÷òî âûáðàííûé èì ïðîãðàììíûé ïðîäóêò ñîîòâåòñòâóåò åãî íóæäàì.

Ïîëüçîâàòåëü íå îïëà÷èâàåò ðàñõîäû ïðîèçâîäèòåëÿ è ïðîäàâöà íà ðåêëàìó, îïëàòó òðóäà ïðîäàâöîâ, àðåíäó òîðãîâûõ ïëîùàäåé è äðóãèå íàêëàäíûå ðàñõîäû. Ýòî îáñòîÿòåëüñòâî íå òîëüêî ïðèâîäèò ê ðàçóìíûì öåíàì íà ïðîãðàììíûå ïðîäóêòû. Â âèä SHAREWARE-ïðîãðàìì îòóò áûòü ðåàëèçîâàíû ïðîâêîû, îáðå÷åííûå íà ïðîâàë â âèäå SOFTWARE èç-çà óçêîé ñïåöèàëèçàöèè, íåçíà÷èòåëüíîñòè ðåøàåìîé çàäà÷è è òîìó ïîäîáíûõ ïðè÷èí.

Ïðîãðàììíûå ïðîäóêòû â âèäå SHAREWARE åñòü ðåàëèçàöèÿ èäåé çíà÷èòåëüíî áîëåå øèðîêîãî êðóãà ëþäåé, íåæåëè êðóã ñîòðóäíèêîâ SOFT-ôèðì (÷üè èäåè, íàäî çàìåòèü, òîæå íå âñåãäà ìîãóò áûòü ðåàëèçîâàíû â âèäå SOFTWARE). Ñëåäîâàòåëüíî, ïðåä ïîëüçîâàòåëåì îêàçûâàåòñÿ áîëåå øèðîêèé àññîðòèìåíò.

Ãëàâíûì íåäîñòàòêîì SHAREWARE-ïðîãðàìì, êàê ïðàâèëî, íàçûâàþò îáñòîÿòåëüñòâî, ÿâëÿþùåéñÿ ïðîãîëåíêîì åãî äîñòîèíñòâ - çà íèì íå ñòîèò êðóïíé ôèðìû ñ ãðîìêèì èìåíåì è òûñÿ÷àìè ðàáîòíèêîâ. ×òî æå, íå áóäåì ñïîðèòü î âêóñàõ - êîìó-òî íðàâèòñÿ ïðîôåññèîð â ðàéîííîé ïîëèêëèíèêå, à êîìó-òî - âèçèò ñåìåéíîãî âðà÷à.

Ñ ðàçâèòèåì ýëåêòðîííûõ êîìóíèêàöèé ñõîäèò íà íåò ïðîáëåìà ïîääåðæêè SHAREWARE - ïðîñòî âìåñòî ãîðÿ÷èõ òåëåôîííûõ Âàì ïðåäëàãàþñÿ WWW èëè E-mail àäðåñà..

Â ñâÿçè ñî ñêàçàííûì õî÷åòñÿ ïðèçâàòü - ðåãèñòðèðóéòåñü! Ïåðå÷èñëÿÿ ðåãèñòðàöèîííûé âçíîñ çà SHAREWARE - ïðîäóêò, Âû íå òîëüêî îïëà÷èâàåòå òðóä àâòîðà êîíêðåòíé ïðîãðàììû è ñòèìóëèðóåòå åãî äëÿ ðàçâèòèÿ âûáðàííé Âàìè ïðîãðàììû, íî è ïîääåðæèâàåòå ñîáñòâåííî ïðèíöèïû SHAREWARE, à ÷òî îíè Âàì äàþò - ñìîòðè âûøå.

Àâòîðàññòàíîâêà êîýôôèöèåíòîâ õèìè÷åñêîãî óðàâíåíèÿ

English

Ýòà ôóíêöèÿ ïðîãðàììû "Õèìè÷åñêèé êàëüêóëÿòîð" âêëþ÷àåòñÿ/âûêëþ÷àåòñÿ ïåðåêëþ÷àòåëåì â ñåðâèñå ÷èæíåé ÷àñòè ãëàâíîãî îêíà. Ïðè âêëþ÷åíèì ñîñòîÿíèè ïåðåêëþ÷àòåëÿ ïðîãðàììà ïûòàåòñÿ ñàìà ðàñ÷èòûâàòü êîýôôèöèåíòû óðàâíåíèÿ (êðîìå áëîêèðîâàííûõCC_Fix). Ðåçóëüòàòû ýòèõ ïîûòîê îòîáðàæàþòñÿ ñïðàâà â íèæíåé ñòðîêå:

- "Ðåøåíèå åäèíñòâåííî" - ðàñ÷åò óñïåøíî çàâåðøåí, åäèíñòâåííî âîçìîæíûé (ñ òî÷íîñòüþ äî òûñÿ÷íûõ äîëåé) íàéäåí êîýôôèöèåíòîâ ðàññòàâëåí â ñîîòâåòñòâóþùèõ ïëÿõ;
- "Ðåøåíèå ÍÅ åäèíñòâåííî" - ðàñ÷åò óñïåøíî çàâåðøåí, íî ìíîæåñòâî ðåøåíèé íå èñ÷åðïûâàåòñÿ îäíèì (ñ òî÷íîñòüþ äî òûñÿ÷íûõ äîëåé) íàéäåíî êîýôôèöèåíòîâ - âîçìîæíû âàðèàíòû, ñâÿçàííûå ñ äðóãèìè ïðîïîðöèÿìè ìåæäó ðåàãåíòàìè. Îäíî èç ðåøåíèé îòîáðàæåíî â ïîëÿõ êîýôôèöèåíòîâ ðåàêöèè;
- "Ðåøåíèå îòñóòñòâóåò" - èñõîäíûå äàííûå íå ïîçâîëÿþò âûïîëíèòü îäíîâðåìåííî âñå óñëîâèÿ áàëàíñà ïî ýëåìåíòàì, ïîëÿ êîýôôèöèåíòîâ îñòàþòñÿ íåèçìåííûìè. Â ýòîì ñëó÷àå ïóòåì ùåë÷êà ëåâîé êëàâèøåé ìûøè íàä èíäèêàòîðîì Âû ìîæåòå ïîëó÷èòü äîñòóï ê îêíó àíàëèçà ïðè÷èí îòñóòñòâèÿ ðåøåíèÿ.

Íå ðàññìàòðèâàÿ ïîäîáíî ìàòåìàòè÷åñêèå ïðè÷èíû îòñóòñòâèÿ èëè ìíîæåñòâåííîñòè ðåøåíèÿ, ïðèâåäåì íåêîòîðûå ïðèìåðû:

$Cu + CuO = Cu_2O$ - решение единственно;

$3Cu + O_2 = Cu_2O + CuO$ - решение НЕединственно;

$CuO + BaO = Cu + Ba$ - решение отсутствует;

Èç ïðîöåññà àâòîðàññòàíîâêè èñêëþ÷àþòñÿ çàáëîêèðîâàííûå êîýôôèöèåíòû. Îîýòîì åñëè Âàñ ïî êàêîé-ëèáî ïðè÷èíå íå óñòðàèâàþò ðåçóëüòàòû àâòîðàññòàíîâêè êîýôôèöèåíòîâ, Âû ìîæåòå ïîäêðóêîèðîâàòü ðåøåíèå, èçìåíÿÿ îäèí èëè íåñêîëüêî êîýôôèöèåíòîâ (ïðè ðåäàêòèðîâàíèè îíè ñòàçó áëîêèðóþòñÿ). Âùå âàðèàíò - ùåëêíèòå ëåâîé êëàâèøåé ìûøè íàä ïåðåêëþ÷àòåëåì àâòîðàññòàíîâêè- ýòî èçìåíèò åãî ñîñòîÿíèå. Ïðè ðàññòàíîâêå êîýôôèöèåíòîâ óðàâíåíèÿ âðó÷íóþ Âàì îæåò ïîìî÷ü èíäèêàòîð ìàòåðèàëüíîãî áàëàíñà (â íèæíåé ñòðîêå ñëåâà). Äëÿ âêëþ÷åíèÿ àâòîðàññòàíîâêè ñíîâà ùåëêíèòå ëåâîé êëàâèøåé ìûøè íàä ïåðåêëþ÷àòåëåì.

Âûáîð íàçâàíèé èç ñïèñêà ñîåäèíåíèé

English

Ñïèñîê ñîåäèíåíèé âûïàäàåò ïðè ùåë÷êå ëåâîé êëàâèøåé ìûøè íàä ëþáûì ïîëåì íàçâàíèÿ â ãëàâíîì îêíå, à òàêæå íàä ïîëÿìè âåùåñòâà è ðàñòâîðèòåëÿ â îêíå ìàñòåðà. Ñïèñîê ñôîðìèðîâàí îòñîðòèðîâàííûì â àëôàâèòíîì ïîðÿäêå ñîäåðæèìûì áàçû äàííûõ (ÁÄ) î õèìè÷åñêèõ ñîåäèíåíèÿõ è ñâåðõó äîïîëíåí (êðîìå ìàñòåðà ðàñòâîðîâ) ïóñòîé ñòðîêîé è ñëóæåáíîé ôðàçîé "Íîâîå ñîåäèíåíèå".

Óæå ïðè íåáîëüøîì ÷èñëå çàïèñåé ÁÄ ñïèñîê íå ïîìåùàåòñÿ öåëèêîì â íåáîëüøîì îòâåäåííîì äëÿ ýòèõ öåëåé îêíøå÷êà. Äëÿ ïðîêðóòêè ñïèñêà èñïîëüçóéòå ïîêíó ïðîêðóòêè èëè êëàâèøè ñî ñòðåëêàìè íà êëàâèàòóðå. ×òîáû ïîäòâåðäèòü âûáîð âûäåëåííîé öåëòî ñòðîêè è çàïèñàòü åå â ñîáñòâåííî ïîëå íàçâàíèÿ, äîñòàòî÷íî íàæàòü êëàâèøó <Enter> íà êëàâèàòóðå èëè ëåâóþ êíîïêó ìûøè íàä ýòîé ñòðîêîé. Ê Âàøèì óñëóãàì òàêæå ïîèñê íàçâàíèÿ â ñïèñêå ïî êëþ÷ó. Âàì äîñòàòî÷íî íàáðàòü íà êëàâèàòóðå íåñêîëüêî ïåðâûõ ñèìâîëîâ íàçâàíèÿ - è êóðñîð áóäåò ïåðåìåùåí íà ñîîòâåòñòâóþùåé ýëåìåíò ñïèñêà. Íàáðàííûå Âàìè ñèìâîëû (êëþ÷ ïîèñêà) ïðè ýòîì âèäíû â ÿðëû÷êå ïîäñêàçêè, à ñîîòâåòſòâóþùèé ýëåìåíò ñïèñêà çàíñèòñÿ â ïîëå íàçâàíèÿ. Îøèáêè ââîäà êëþ÷à îïãóò áûòü èñïðàâëåíû êëàâèøàìè <Backspace> (óäàëåíèå ïîñëåäíåãî ñèìâîëà èç êëþ÷à) è <Esc> (ñáðîñ âñåãî ñîäåðæèìîãî êëþ÷à).

Âûáîð ñëóæåáíîé ôðàçû "Íîâûå ñîåäèíåíèå" àêòèâèçèðóåò ñïåöèàëüíîå îêíî ðåäàêòèðîâàíèÿ íîâîé çàïèñè ÁÄ. Åñëè ðåäàêòèðîâàíèå ïîëé ýòîãî îêíà Âû çàâåðøèòå íàæàòèåì êíîïêè "Ok" (â íèæíåé ÷àñòè îêíà ñëåâà), òî íîâàÿ çàïèñü áóäåò ñîõðàíåíà â ÁÄ, à íàçâàíèå íîâîãî ñîåäèíåíèÿ ñðàçó ïîïàäåò â òî ïîëå íàçâàíèÿ, äëÿ êîòîðîãî äåëàëñÿ âûáîð.

Âûáîð ïóñòîé ñòðîêè (â ñàìîì âåðõó ñïèñêà) ñëóæèò äëÿ èñêëþ÷åíèÿ ñòðîêè òàáëèöû â ãëàâíîì îêíå èç õèì÷åñêîãî óðàâíåíèÿ. Îíæíî î÷èñòèòü ñðàçó âñå ïîëÿ, åñëè âûáðàòü ïóíêò "Î÷èñòèòü" îñíîâíîãî ìåíþ.

ßçûê ïîëüçîâàòåëüñêîãî èíòåðôåéñà

English

Âîçìîæíîñòü ñìåíû ÿçûêà îáùåíèÿ ïîëüçîâàòåëÿ ñ ïðîãðàììîé ïîÿâèëàñü â âåðñèè 1.5 Õèì÷åñêîãî Êàëüêóëÿòîðà. Ïåðå÷åíü âîçìîæíûõ ÿçûêîâ äëÿ èñïîëüçóåìîé Âàìè âåðñèè Âû ìîæåòå íàéòè â ôàéëå history.*. Ïåðåêëþ÷åíèå ÿçûêîâ îñóùåñòâëÿåòñÿ â ïóíêòå **Language** îñíîâíîãî ìåíþ ãëàâíîãî îêíà. Îäíàêî äëÿ óñïåõà íåîáõîäèìî òàêæå íàëè÷èå â ñèñòåìå øðèôòîâ (íå îáÿçàòåëüíî âñåõ, íî ñèñòåìíûõ - îáÿçàòåëüíî) ñ íàöèîíàëüíûì àëôàâèòîì. Åñëè âû ïîëüçóåòåñü ëîêàëèçîâàííîé âåðñèåé WINDOWS, òî îíè ó Âàñ óæå åñòü.

Ñïðàâî÷íèê, êîòîðûé Âû ñåé÷àñ ÷èòàåòå, ñîäåðæèò èíôîðìàöèþ äëÿ ïðîãðàììû ñ âûáðàííûì ðóññêèì ÿçûêîì. Â âåðõíåé ÷àñòè êàæäîé ñòðàíèöû ñïðàâî÷íèêà, ïîëíûé èëè ÷àñòè÷íûé ýêâèâàëåíò êîòîðîé èìåþòñÿ íà äðóãèõ ÿçûêàõ, èìåþòñÿ ññûëêè íà ýòè ÿçûêè. Ðóññêèé âàðèàíò ñïðàâî÷íèêà íàèáîëåå ïîëíûé, ïîñêîëüêó ýòî ðîäíîé ÿçûê àâòîðà ïðîãðàììû.

Áëîêèðîâàíèå êîýôôèöèåíòîâ

English

Âîçìîæíîñòü áëîêèðîâàíèÿ ÷àñòè êîýôôèöèåíòîâ óðàâíåíèÿ ðåãðåññèè ïðè àâòîðåãðåññèîííîé îøèáêå â âåðñèè 1.6 Õèè÷åñêîãî Êàëüêóëÿòîðà. Äîñòóï ê ôóíêöèè áëîêèðîâàíèÿ/ðàçáëîêèðîâàíèÿ îñóùåñòâëÿåòñÿ ÷åðåç ìåíþ, âñïëûâàþùåå ïðè íàæàòèè ïðàâîé êíîïêè ìûøè íàä ïîëåì ñîîòâåòñòâóþùåãî êîýôôèöèåíòà. Êðîìå òîãî, êîýôôèöèåíòû áëîêèðóþòñÿ àâòîìàòè÷åñêè ïðè ðåãðåññèîííîì àíàëèçå âðó÷íóþ. Áëîêèðîâàííûå êîýôôèöèåíòû èìåþò ôîí ãîëóáîãî öâåòà, ñâîáîäíûå - áåëîãî.

Ïåðâîíà÷àëüíîé öåëüþ ýòîãî íîâîââåäåíèÿ áûëî îáëåã÷åíèå ðàñ÷åòà íàâåñîê äëÿ ñèíòåçà ñîñòàâà, ïîðåäåëÿåìîãî ïåðåñ÷åíàì äâóõ îòðåçêîâ âíóòðè ôàçîâîé äèàãðàììû òðîéíîé ñèñòåìû (òðåóãîëüíèêà). Ýòàï ïîðåäåëåíèÿ ñîñòàâà òî÷êè ïåðåñ÷åíèÿ ïðîïîðöèîíàëåí ëåãêî - äîñòàòî÷íî áûëî çàïèñàòü â ëåâóþ è ïðàâóþ ÷àñòè óðàâíåíèÿ òå ñîäåèíåíèÿ, ÷òî ëåæàò íà êîíöàõ îòðåçêîâ. Ïðîãðàììà àâòîìàòè÷åñêè ðàñïòàâëÿåò êîýôôèöèåíòû, ïîñëå ÷åãî îäíó èç ÷àñòåé óðàâíåíèÿ ïðèðîâíèñü çàïèñûâàòü â ÁÄ êàê áèíàðíûé ðàñòâîð ñ öåëüþ çàôèêñèðîâàòü ïîëó÷åííûå ñîîòíîøåíèÿ (òî÷êó íà îòðåçêå). È òîëüêî ïîñëå ýòîãî íîâîå ñîåäèíåíèå áûëî âîçìîæíî àâòîìàòè÷åñêè ñîñòàâèòü èç èìåþùèõñÿ â íàëè÷èè ðåàêòèâîâ (íáû÷íî âåðøèí òðåóãîëüíèêà). Òåïåðü ìîæíî, íå çàõîäÿ ÁÄ, çàôèêñèðîâàòü ïîëó÷åííûå íà ïåðâîì ýòàïå êîýôôèöèåíòû ïðÿìî â ãëàâíîì çàìåíòü îäíó èç ÷àñòåé óðàâíåíèÿ íà èìåþùåéñÿ ðåàêòèâû, íå âûêëþ÷àÿ àâòîðåãðåññèîííîé.

Åñëè Âû íàéäåòå äðóãèå ñîîñíîâû ïðèìåíåíèÿ áëîêèðîâêè, ïîäåëèòåñü èìè ñ êîëëåãàìè è ðàçðàáîò÷èêîì ïðîãðàììû.

Ðåãèñòðàöèîííàÿ ôîðìà

English

×òîáû çàïîëíèòü, ñêîïèðóéòå â êàêîé-ëèáî ðåäàêòîð.
Çàïîëíèâ, ïîñûëàéòå ïî ýëåêòðîííîé ïî÷òå.
Äëÿ èìåþùèõ âûõîä â Internet åñòü è äðóãîé ìåòîä -
http://www.geocities.com/SiliconValley/Bay/7132/regform.html

To: lakhtin@hotmail.com
Subject: Õèì÷åñêèé êàëüêóëÿòîð

"Õèì÷åñêèé êàëüêóëÿòîð" - Ðåãèñòðàöèîííàÿ ôîðìà

Ôàìèëèÿ, Èìÿ, Îò÷åñòâî _____

Îðãàíèçàöèÿ (íåîáÿçàòåëüíî):_____

E-mail (îáÿçàòåëüíî): _____

ß ïîëó÷èë Õèì÷åñêèé êàëüêóëÿòîð _____ (íîìåð âåðñèè - íåîáÿçàòåëüíî)

èç ñëåäóþùåãî èñòî÷íèêà:_____ (íåîáÿçàòåëüíî)

ß õî÷ó çàðåãèñòðèðîâàòü ____ êîïèé ïðîãðàììû "Õèì÷åñêèé êàëüêóëÿòîð"

äëÿ èñïîëüçîâàíèÿ_____ (íà êîìàíäíûé êîìïüþòåð / â ñåòè)

â îáëàñòè _____

_____
(îáðàçîâàíèÿ, íàóêè, ïðîìûøëåííîñòè è ò.ï. - íåîáÿçàòåëüíî)

ß ïðåäïî÷èòàþ ïîëàòèòü ðåãèñòðàöèîííûé âçíîñ â ôîðìå_____

_____

Registration Form

Ðóññêèé

For WWW users: fill the form at
http://www.geocities.com/SiliconValley/Bay/7132/regform.html
For other: Copy to any word processor, fill and send by E-mail.

To: lakhtin@hotmail.com
Subject: Ural Chemical Calculator

Ural Chemical Calculator Registration Form

Your Full Name: _____

Organization (optional):_____

E-mail (required):_____

I have got the UrChemCalc v._____ (number of version - optional)

from _____ (source of copy - optional)

I would like to register _____ copy / (copies) of UrChemCalc to use it

_____ (at local PC / in net) in the field(s) of

_____

_____
(education, scientific research, industry, etc. - optional)

Ñîäåðæàíèå ñïðàâêè

English

Âûáåðèòå èíòåðåñóþùóþ Âàñ òåìó èç ïåðå÷èñëåííûõ íèæå îñíîâíûõ ðàçäåëîâ ñïðàâêè:

Íàçíà÷åíèå ïðîãðàììû "Õèìè÷åñêèé êàëüêóëÿòîð"

English

Ïðîãðàììà ïðåäíàçíà÷åíà äëÿ ðàñ÷åòîâ ìàññ èñõîäíûõ âåùåñòâ è ïðîäóêòîâ õèìè÷åñêèõ ðåàêöèé ïî ïîëíîñòüþ èëè ÷àñòè÷íî èçâåñòíîìó óðàâíåíèþ ðåàêöèè. Ïîäîáíûå çàäà÷è íåðåäêî âîçíèêàþò êàê ó õèìèêîâ-ñèíòåòèêîâ, òàê è ó õèìèêîâ-àíàëèòèêîâ. Ñ ìàòåìàòè÷åñêîé òî÷êè çðåíèÿ îíè â îñíîâíîì ñâîäÿòñÿ ê ïðîñòûì ëèíåéíûì ïðåîáðàçîâàíèÿì ìåæäó ìîëüíûìè è ìàññîâûìè ïðîïîðöèÿìè. Àâòîðó èçâåñòíû íåñêîëüêî áîëåå èëè ìåíåå ðàñïðîñòðàíåííûõ ìåòîäîâ, äî ñèõ ïîð ïðèìåíÿâøèõñÿ õèìèêàìè äëÿ ðåøåíèÿ ïîäîáíûõ çàäà÷: íà ñàëôåòêå ñòîëáèêîì (â ïîñëåäíåå âðåìÿ ñ÷èòàåòñÿ óñòàðåâøèì), â óíèâåðñàëüíûõ ýëåêòðîííûõ òàáëèöàõ (íà ýòîò ïîâîä ñïîñîáíû íåìíîãèå), à òàêæå ïðè ïîìîùè êàëüêóëÿòîðà. Ñðåäè îñíîâíûõ îòëè÷èé îïèñûâàåìîé ïðîãðàììû îò àíàëîãè÷íûõ ðàñ÷åòîâ, ïðîèçâîäèìûõ íà êàëüêóëÿòîðå, ìîæíî âûäåëèòü:

- ïîääåðæêà áàçû äàííûõ î õèìè÷åñêèõ ñîåäèíåíèÿõ;
- ñêðûòûé ðàñ÷åò ìîëÿðíûõ ìàññ õèìè÷åñêèõ ñîåäèíåíèé;
- àâòîìàòè÷åñêàÿ ïðîâåðêà óðàâíåíèÿ ðåàêöèè;
- àâòîìàòè÷åñêèé ðàñ÷åò êîýôôèöèåíòîâ óðàâíåíèÿ ðåàêöèè;
- âîçìîæíîñòü âûâîäà ðåçóëüòàòà ðàñ÷åòà íà ïðèíòåð èëè â äðóãèå WINDOWS-ïðèëîæåíèÿ.

Íî çà âñå íóæíî ïëàòèòü - è ïðîãðàììà òðåáóåò êîìïüþòåðà ñ WINDOWS íå íèæå 3.1, óñòàíîâëåííîãî DataBase Engine è ñàìà çàíèìàåò îêîëî ìåãàáàéòà íà æåñòêîì äèñêå (ìîæíî ðàáîòàòü è ñ ãèáêîãî - íî ñêîðîñòü íåêîòîðûõ îïåðàöèé òðóäíî áóäåò íàçûâàòü ñêîðîñòüþ).

Ïðåäïîëàãàåìûé ïóòü èñïîëüçîâàíèÿ ïðîãðàììû - ââîä óðàâíåíèÿ ðåàêöèè (â ãëàâíîì îêíå), çàäàíèå ìàññû îäíîãî èç ðåàãåíòîâ (ïðîãðàììà ñðàçó ïîäñ÷èòàåò ìàññû îñòàëüíûõ) è, âåðîÿòíî, ïå÷àòü ðåçóëüòàòà. Åñëè Âû íàéäåòå äðóãîå ïðèìåíåíèå ïðîãðàììû, àâòîð áóäåò òîëüêî ðàä.

Ãëàâíîå îêíî ïðîãðàììû

English

Ãëàâíîå îêíî ïîÿâëÿåòñÿ ñðàçó ïîñëå çàãðóçêè ïðîãðàììû è ñîäåðæèò íåêîå ïîäîáíå òàáëèöû, ñòîëáöû êîòîðîé ñîîòâåòñòâóþò èç ðåäàêòèðóåìûõ ïîëåé ðàçëè÷íûõ âèäîâ:

- ÷èñëîâûå ïîëÿ äëÿ êîýôôèöèåíòîâ óðàâíåíèÿ ðåàêöèè (ìîãóò áûòü íåöåëî÷èñëåííûìè);
- ïîëÿ íàçâàíèé èñõîäíûõ âåùåñòâ (ñëåâà) è ïðîäóêòîâ ðåàêöèè (ñïðàâà), çàïîëíÿåìûå ïóòåì âûáîðà èç ñïèñêà, âûïàäàþùåãî ïðè íàæàòèè íà êíîïêó ñî ñòðåëêîé â ïðàâîé ÷àñòè ïîëÿ;
- ïîëÿ çíà÷åíèé ìàññû, îäíî èç êîòîðûõ (ïîñëåäíåå èçìåíåííîå) îáû÷íî âûäåëåíî öâåòîì è ñëóæèò èñõîäíîé âåëè÷èíîé äëÿ ðàñ÷åòà, à îñòàëüíûå çàïîëíÿþòñÿ àâòîìàòè÷åñêè è ïî ñóòè ÿâëÿþñÿ ðåçóëüòàòîì âû÷èñëåíèé.

Â íèæíåé ÷àñòè ãëàâíîãî îêíà íàõîäÿòñÿ (ñëåâà íàïðàâî): èíäèêàòîð ïîëíîòû ââåäåííîãî óðàâíåíèÿ ðåàêöèè ("Ìàòåðèàëüíûé áàëàíñ ÏÎËÍÛÉ/ÍÅÏÎËÍÛÉ"), ïåðåêëþ÷àòåëü êîýôôèöèåíòîâ óðàâíåíèÿ è (ïðè âêëþ÷åíîé àâòîðàññòàíîâêå) èíäèêàòîð åäèíñòâåííîñòè íàáîðà êîýôôèöèåíòîâ. Â âåðõíåé ÷àñòè ðàñïîëîæåíî ìåíþ äëÿ äîñòóïà ê ñëåäóþùèì ôóíêöèÿì ïðîãðàììû:

- **Language**- âûáîð ÿçûêà ïîëüçîâàòåëüñêîãî èíòåðôåéñà ïðîãðàììû;
- **ÁÄ î ñîåäèíåíèÿõ** - ðåäàêòèðîâàíèå áàçû äàííûõ î õèì÷åñêèõ ñîåäèíåíèÿõ;
- **Ïå÷àòü** - âûâîä ðåçóëüòàòà ðàñ÷åòà íà ïðèíòåð èëè â äðóãîå WINDOWS-ïðèëîæåíèå ñ ïðåäâàðèòåëüíûì ïðîñìîòðîì íà ýêðàíå;
- **Î÷èñòêà** - ñáðîñ òåêóùåãî óðàâíåíèÿ, î÷èñòêà âñåõ ïîëåé ãëàâíîãî îêíà;
- **Ñïðàâêà** äàåò äîñòóï
    - ê îêíó WINDOWS HELP, â êîòîðîì âû âñå ýòî ñåé÷àñ è ÷èòàåòå,
    - ê îêíó êðàòêîé èíôîðìàöèè î ïðîãðàììå,
    - ê äîìàøíåé ñòðàíè÷êå ïðîãðàììû (åñëè óñòàíîâëåí WWW-íàâèãàòîð),
    - ê ôîðìå ñîñòàâëåíèÿ ñîîáùåíèé ðàçðàáîò÷èêó ïðîãðàììû (òîæå ÷åðåç Internet),
    - ê îêíó ðåãèñòðàöèè ïðîãðàììû (åñëè îíà íå çàðåãèñòðèðîâàíà);
- **Exit** - çàêðûòèå îêíà, îêîí÷àíèå ðàáîòû ñ ïðîãðàììîé.

Êðîìå òîãî, ãëàâíîå îêíî ñîäåðæèò êîìïîíåíòû ñòàíäàðòíîãî îêíà WINDOWS - êíîïêó ñèñòåìíîãî ìåíþ è êíîïêè óïðàâëåíèÿ ðàçìåðîì, à òàêæå çàãîëîâîê ñ óêàçàíèåì íîìåðà âåðñèè ïðîãðàììû.

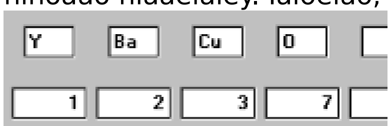
Áàçà äàííûõ î õèìè÷åñêèõ ñîåäèíåíèÿõ

English

Íàçíà÷åíèå ýòîé áàçû äàííûõ (ÁÄ) - õðàíåíèå èíôîðìàöèè îá ýëåìåíòíîì ñîñòàâå õèìè÷åñêèõ ñîåäèíåíèé. Ôèçè÷åñêè õðàíèòñÿ â ôàéëàõ OUR.*. Äîïóñêàåò ðàñøèðåíèå ñòðóêòóðû, íî íå óäàëåíèå èëè ïåðåèìåíîâàíèå ñëóæåáíûõ ïîëåé. Äîñòóï ê ðåäàêòèðîâàíèþ ÁÄ â ïðîãðàììå ðåàëèçîâàí äâóìÿ ñïîñîáàìè:

- ÷åðåç âûáîð ñëóæåáíîé ôðàçû "Íîâîå ñîåäèíåíèå" â âûïàäàþùåì ñïèñêå ëþáîãî ïîëÿ íàçâàíèÿ â ãëàâíîì îêíå. Â ýòîì   ñëó÷àå ïðåäëàãàåòñÿ çàïîëíèòü íîâóþ çàïèñü ÁÄ;

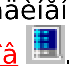
- ÷åðåç âûáîð ïóíêòà "ÁÄ î ñîåäèíåíèÿõ" îñíîâíîãî ìåíþ â ãëàâíîì îêíå. Â ýòîì ñëó÷àå äîñòóïíû äëÿ ðåäàêòèðîâàíèÿ âñå çàïèñè ÁÄ, âîçìîæíî òàêæå óäàëåíèå è äîáàâëåíèå îòäåëüíûõ çàïèñåé. Îòêðûâàþùååñÿ îêíî ñîäåðæèò ñïèñîê íàçâàíèé ñîåäèíåíèé, ñëóæàùèé êàê äëÿ ïåðåìåùåíèÿ ïî ÁÄ (òåêóùàÿ çàïèñü âûäåëåíà öâåòîì è óêàçàòåëåì) òàê è äëÿ ðåäàêòèðîâàíèÿ íàçâàíèé "ïî ìåñòó". Ïîä ñïèñêîì íàçâàíèé ðàñïîëîæåíû íåñêîëüêî ïàð ïîëåé ýëåìåíò-êîýôôèöèåíò, òîíîñÿùèåñÿ ê òåêóùåé çàïèñè. Ñîäåðæèìîå ýòèõ ïîëåé äîëæíî ñîîòâåòñòâîâàòü ýëåìåíòíîìó ñîñòàâó ñîåäèíåíèÿ. Íàïðèìåð, äëÿ ñîåäèíåíèÿ YBa2Cu3O7 ýòî ìîæåò âûãëÿäåòü òàê:



Êîýôôèöèåíòû ìîãóò áûòü íåöåëî÷èñëåííûìè, åñëè ýòî íåîáõîäèìî äëÿ ó÷åòà íåñòåõèîìåòðèè, îïèñàíèÿ ðàñòâîðîâ è ò.ï.. Ïðîãðàììà íå íàêëàäûâàåò ñåðüåçíûõ îãðàíè÷åíèé íà íàçâàíèå ñîåäèíåíèÿ, íî ðåêîìåíäóåòñÿ:
- îòðàæàòü â íàçâàíèè òó ôîðìóëó, êîòîðàÿ ñîîòâåòñòâóåò ñîäåðæèìîìó ïîëåé ýëåìåíòû-êîýôôèöèåíòû,
- íå ïîâòîðÿòü íàçâàíèé â ðàçíûõ çàïèñÿõ (èíà÷å Âû íå ðàçëè÷èòå èõ â ñïèñêàõ),
- íå èñïîëüçîâàòü ñëóæåáíóþ ôðàçó "Íîâîå ñîåäèíåíèå" â êà÷åñòâå íàçâàíèÿ ñîåäèíåíèÿ.

Åñëè ïðè ðåäàêòèðîâàíèè çàïèñè ÁÄ íàçâàíèå îñòàëîñü ïóñòûì, ïðîãðàììà ñàìà äàñò åìó èíäèâèäóàëüíîå íàçâàíèå, ïîïûòàâøèñü ñîñòàâèòü ôîðìóëó èç ñîäåðæèìîãî ïîëåé ýëåìåíòû è êîýôôèöèåíòû. È íàîáîðîò, åñëè ïóñòûå ïîëÿ ýëåìåíòû è êîýôôèöèåíòû, íî íå ïóñòîå íàçâàíèå, ïðîãðàììà ïîïûòàåòñÿ çàïîëíèòü ïîëÿ, òðàêòóÿ íàçâàíèå êàê ôîðìóëó. Åñëè âñå ïîëÿ ïóñòû, çàïèñü áóäåò àâòîìàòè÷åñêè óäàëåíà èç ÁÄ. Åñëè â ÁÄ ïîÿâèëèñü äóáëèðóþùèå íàçâàíèÿ, ïðîãðàììà áóäåò òî è äåëî íàïîìèíàòü îá ýòîì. Êîãäà Âàì ýòî íàäîåñò, âåðíèòåñü ê ðåäàêòèðîâàíèþ ÁÄ è ëèáî óäàëèòå äóáëèðóþùóþ çàïèñü, ëèáî ñìåíèòå åå íàçâàíèå. Íàèáîëåå ïðîñòîé (íî íå âñåãäà ëó÷øèé) ñïîñîá ñîñòàâëåíèÿ íàçâàíèÿ ïðåäëàãàåòñÿ Âàì â âèäå êíîïêè  ñëåâà îò ïîëåé ýëåìåíòîâ. Â ñëó÷àå íàæàòèÿ ýòîé êíîïêè ïðîãðàììà ñîñòàâèò íàçâàíèå ñîåäèíåíèÿ èç ñîäåðæèìîãî ïîëåé ýëåìåíòîâ è êîýôôèöèåíòîâ. Ïðè íåîáõîäèìîñòè äîïîëíèòå èëè îòðåäàêòèðóéòå ýòî íàçâàíèå. Îáðàòíîå äåéñòâèå - çàïîëíåíèå ïîëåé ýëåìåíòîâ è êîýôôèöèåíòîâ èç íàçâàíèÿ ïðîèçâîäèòñÿ ïðè íàæàòèè êíîïêè

 , íî äëÿ ýòîãî íàçâàíèå äîëæíî ïðåäñòàâëÿòü èç ñåáÿ õèìè÷åñêóþ ôîðìóëó ñîåäèíåíèÿ.

Òàêæå ñëåâà íàõîäèòñÿ åùå îäíà êíîïêà - êíîïêà âûçîâà ìàñòåðà ðàñòâîðîâ  . Áóäüòå âíèìàòåëüíû - ìàñòåð çàïîëíÿåò **òåêóùóþ çàïèñü ÁÄ**! Åñëè ðàñòâîð äîëæåí áûòü çàïèñàí â äîïîëíåíèå ê óæå ñóùåñòâóþùèì çàïèñÿì, ïåðåä âûçîâîì ìàñòåðà íå çàáóäüòå íàæàòü êíîïêó **Âñòàâêà**.

Ïðîãðàììà íå òîëüêî ñëåäèò çà ïðàâèëüíîñòüþ çàïîëíåíèÿ ïîëåé ýëåìåíòîâ, íî è ïðåäëàãàåò äëÿ ýòîãî çàâåäîìî ñâîáîäíûé îò îðôîãðàôè÷åñêèõ îøèáîê ïóòü - âûáîð èç ïåðèîäè÷åñêîé òàáëèöû. Òàáëèöà ïîÿâëÿåòñÿ íà äâîéíîé ùåë÷îê ëåâîé êíîïêîé ìûøè íàä ïîëåì ýëåìåíòà èëè ïðè âûáîðå ñîîòâåòñòâóþùåãî ïóíêòà ìåíþ, âñïëûâàþùåãî ïðè íàæàòèè ïðàâîé êíîïêè ìûøè íàä ïîëåì. Âûáðàííûé â òàáëèöå ýëåìåíò ïðîãðàììà àâòîìàòè÷åñêè çàíîñèò â ïîëå â ïðàâèëüíîé íîòàöèè (ýòà ïðàâèëüíîñòü îïðåäåëÿåòñÿ ñîäåðæèìûì ÁÄ î õèìè÷åñêèõ ýëåìåíòàõ).

Ñïðàâà ðàñïîëîæåíî ïîëå ìîëÿðíîé ìàññû. Îíî íå ïîäëåæèò ðåäàêòèðîâàíèþ, íî Âû ìîæåòå, âûäåëèâ åãî ñîäåðæèìîå, ñêîïèðîâàòü åãî â Áóôåð Îáìåíà WINDOWS (íàïðèìåð, êëàâèøàìè <Ctrl><C>) äëÿ ïîñëåäóþùåãî èñïîëüçîâàíèÿ äðóãèìè ïðîãðàììàìè.

Äâîéíîé ùåë÷îê ëåâîé êíîïêîé ìûøè íàä ïîëåì êîýôôèöèåíòà (åñëè îíî çàïîëíåíî) îòêðûâàåò âîçìîæíîñòü ðàçäåëèòü âñå êîýôôèöèåíòû ôîðìóëû íà îäíî ÷èñëî, ïðè÷åì â êà÷åñòâå

çàòðàâî÷íîãî çíà÷åíèÿ äåëèòåëÿ ïðåäëàãàåòñÿ çíà÷åíèå êîýôôèöèåíòà â âûáðàííîì ïîëå. Íàïðèìåð, ÷òîáû ïðèâåñòè ôîðìóëó Li20Ni19FeO40 ê âèäó LiNi0.95Fe0.05O2, ìîæíî äâàæäû ùåëêíóòü íàä ïîëåì êîýôôèöèåíòà ïðè Li è â ïîÿâèâøåìñÿ îêíøêå ïîäòâåðäèòü æåëàíèå ðàçäåëèòü ôîðìóëó íà 20, íàæàâ êíîïêó Ok. Â ïðèâåäåííîì ïðèìåðå Âû ìîãëè áû è âðó÷íóþ ââåñòè íåîáõîäèìûå çíà÷åíèÿ êîýôôèöèåíòîâ è ïîëíàííûé ïðèì ëèøü ñýêîíîìèë Âàøå âðåìÿ. Íàèáîëüøóþ æå ïîëüçó äàííûé ïðèì ñîïðîâîæ ïðèíåñòè â ñëó÷àå ïðèâåäåíèÿ ôîðìóë, ïîëó÷åííûõ ñ ïîìùüþ ìàñòåðà ðàñòâîðîâ, ïîñêîëüêó îí íå ñíèæàåò òî÷íîñòè êîýôôèöèåíòîâ â îòëè÷èå îò ðåäàêòèðîâàíèÿ âðó÷íóþ.

Â íèæíåé ÷àñòè îêíà "Ábàçà äàííûõ î õèì÷åñêèõ ñîåäèíåíèÿõ" íàõîäÿòñÿ êíîïêè óïðàâëåíèÿ:
Ok - ïîäòâåðæäåíèå ïîñëåäíèõ èçìåíåíèé è çàêðûòèå îêíà, âîçâðàùåíèå â ãëàâíîå îêíî,
Cancel - îòìåíà ïîñëåäíèõ èçìåíåíèé â òåêóùåé çàïèñè ÁÄ è çàêðûòèå îêíà, âîçâðàùåíèå â ãëàâíîå îêíî,
Help - âûçîâ îêíà ñïðàâêè, â êîòîðîì Âû âñå ýòî ñåé÷àñ ÷èòàåòå,
Âñòàâêà - äîáàâëåíèå íîâîé çàïèñè â ÁÄ è ïåðåõîä ê åå çàïîëíåíèþ,
Óäàëèòü - óäàëåíèå òåêóùåé çàïèñè èç ÁÄ. Íà ýòó àêöèþ çàïðàøèâàåòñÿ ïîäòâåðæäåíèå.

Áàçà äàííûõ î õèìè÷åñêèõ ýëåìåíòàõ

English

Íàçíà÷åíèå ýòîé áàçû äàííûõ (ÁÄ) - õðàíåíèå èíôîðìàöèè îá àòîìíûõ âåñàõ õèìè÷åñêèõ ýëåìåíòîâ, èõ ïðàâèëüíîé íîìåíêëàòóðû è ðàñïîëîæåíèè â ïåðèîäè÷åñêîé òàáëèöå. Ôèçè÷åñêè õðàíèòñÿ â ôàéëàõ MENDELEV.*. Äîïóñêàåò ðàñøèðåíèå ñòðóêòóðû, íî íå óäàëåíèå èëè ïåðåìåíîâàíèå ñëóæåáíûõ ïîëé. Äîñòóï ê ðåäàêòèðîâàíèþ ÁÄ â ïðîãðàììå íå ðåàëèçîâàí, îäíàêî îí ìîæåò áûòü ïîëó÷åí èç äðóãèõ ïðîãðàìì. Èìåííî îò ýòîãî è õî÷åòñÿ ïðåäîñòåðå÷ü - íå èçìåíÿéòå áåç êðàéíåé íåîáõîäèìîñòè ñîäåðæèìîå ýòîé ÁÄ! Îíî î÷åíü âàæíî äëÿ ïðàâèëüíîé ðàáîòû ïðîãðàììû "Õèìè÷åñêèé êàëüêóëÿòîð". Çíà÷åíèÿ àòîìíûõ âåñîâ èñïîëüçóþòñÿ äëÿ ðàñ÷åòà ìîëÿðíûõ ìàññ ñîåäèíåíèé, âêëþ÷åííûõ â óðàâíåíèå õèì÷åñêîé ðåàêöèè. Íîòàöèÿ èñïîëüçóåòñÿ â êîíòðîëå ïðàâèëüíîñòè çàïîëíåíèÿ ïîëé ýëåìåíòîâ â ÁÄ î õèì÷åñêèõ ñîåäèíåíèÿõ. Ìåñòîïîëîæåíèå ýëåìåíòà â îêíå ïåðèîäè÷åñêîé òàáëèöû, ïðèçâàííîé ïîìî÷ü ïðè çàïîëíåíèè ïîëé ýëåìåíòîâ, òàêæå îïðåäåëÿåòñÿ ñîäåðæàíèåì ýòîé ÁÄ.

Ïå÷àòü ðåçóëüòàòà

English

Ýòà ôóíêöèÿ ïðîãðàììû "Õèìè÷åñêèé êàëüêóëÿòîð" äîñòóïíà ÷åðåç ïóíêò **Ïå÷àòü** îñíîâíîãî ìåíþ ãëàâíîãî îêíà. Ñîáñòâåííî ïå÷àòè ïðåäøåñòâóåò ïðåäâàðèòåëüíûé ïðîñìîòð ïðîâåðèòå ðàñïå÷àòêè â îêíå ïå÷àòè. Ðàçâåòâëåíèå ìåíþ ýòîãî îêíà ïîìîæåò Âàì âûáðàòü íàèáîëåå ïîäõîäÿùåå ïðåäñòàâëåíèå ðåçóëüòàòà (ïóíêò ìåíþ **Ôîðìà**) è âûáðàòü è íàñòðîèòü ïðèíòåð (**Âûâîä\Íàñòðîéêà_ïðèíòåðà**). Íåò ñìûñëà ïîäðîáíî îïèñûâàòü çäåñü äåéñòâèå îòäåëüíûõ ïîäïóíêòîâ ìåíþ, ïîñêîëüêó âñå èçìåíÿåìî òóò æå îòðàæàþòñÿ â îêíå íà ïðîòÿçå áóäóùåé ðàñïå÷àòêè, êîòîðûé Âû ìîæåòå ðàñïîëîæèòü â ðàçíûõ ìàñøòàáàõ (**Ìàñøòàá_ïðîñìîòðà**). Îòìåòèì ëèøü íåêîòîðûå ìîìåíòû.

Äëÿ òåõ, êòî ïîëüçóåòñÿ íå òàðèôíûìè âåñàìè è âûíóæäåí äîâàâëÿòü ïîñòîÿííûå ñìåùåíèå (âåñ ïîñóäû, ñìåùåíèå íóëÿ âåñîâ è ò.ï.) ê òðåáóåìîé ìàññå, ìîæåò îêàçàòüñÿ ïîëåçíûì ïóíêò ìåíþ **Ôîðìà\Ïðèáàâèòü_âåñ_ïîñóäû**. Âûáîð ýòîãî ïóíêòà ïîçâîëÿåò äîáàâèòü ê òàáëèöå êîëîíêó, â êîòîðîé áóäóò ïå÷àòàòüñÿ ìàññû ñ çàäàííîé Âàìè ïîïðàâêîé.

Âûâîä ïðîòîêîëà âîçìîæåí íå òîëüêî íà ïðèíòåð. Ïóíêò ìåíþ **Âûâîä** ñîäåðæèò ãðóïïó êîìàíä âûâîäà â Áóôåð Îáìåíà WINDOWS (Clipboard) â ðàçëè÷íûõ ôîðìàòàõ. Ïîñëå âûïîëíåíèÿ òàêîé êîìàíäû Âû ìîæåòå ïåðåêëþ÷èòüñÿ íà äðóãîå WINDOWS-ïðèëîæåíèå è âñòàâèòü â íåãî ñîäåðæèìîå Áóôåðà Îáìåíà (êëàâèøàìè <Ctrl><V> èëè <Shift><Ins> è ò.ï., êîìàíäàìè ìåíþ ýòîãî ïðèëîæåíèÿ èëè êîìàíäîé ìåíþ, âñïëûâàþùåãî ïðè íàæàòèè ïðàâîé êíîïêè ìûøè). ÂÍÈÌÀÍÈÅ! Áóôåð Îáìåíà WINDOWS íå ìîæåò ñîäåðæàòü áîëåå îäíîãî îáúåêòà è êàæäûé âûâîä ïðîòîêîëà â íåãî ñòèðàåò ïðåäûäóùåå ñîäåðæèìîå Áóôåðà.

Åñëè Âû óáåäèëèñü, ÷òî ïå÷àòàòüñÿ áóäåò èìåííî òî, î ÷åì Âû äàâíî ìå÷òàëè, è òàì, ãäå ýòî Âàì íóæíî, âûáèðàéòå ïóíêò ìåíþ **Âûâîä\Ïå÷àòü**. Åñëè ðåøèëè íå ïå÷àòàòü - âûáèðàéòå ïóíêò ìåíþ **Exit** è Âû âåðíåòåñü â ãëàâíîå îêíî.

Åñëè Âàøà êîïèÿ ïðîãðàììû íå çàðåãèñòðèðîâàíà, âîçìîæíîñòè âûâîäà íà ïðèíòåð è â Áóôåð Îáìåíà îòñóòñòâóþò. Ðåãèñòðèðóéòåñü!

Input the chemical reaction equation

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The equation is placed in the main window in the form of a table. Two groups with three columns at each correspond to the reagents (the left group) and products (the right group). Two fields describe each term of the chemical equation in this formalism. They are the field of compound name and the field of equation coefficient. These two fields are placed at the same line of the same group. In order to report the result of program work (mass proportions) there is third field near this pair - the mass field. Therefore, each group contains three columns.

To input of equation, choose compound names (both reagents and products). If the Autocalculation of coefficients is turned off, equation coefficients must be entered. If the Autocalculation of coefficients is turned on, Ural Chemical Calculator calculates all free coefficients automatically. In this case the editing of any coefficient field fixes the value of the coefficient and field will be aqua. Fixing or making the coefficient free is also available by way of popup menu. Free fields are white.

Example: Usual form of chemical reaction equation is

$$12CuO+8BaO+2Y_2O_3+O_2 = 4YBa_2Cu_3O_7$$

In UrChemCalc formalism it looks as

Coeff.	Reagents	Masses	Coeff.	Products	Masses
12	CuO		4	$YBa_2Cu_3O_7$	
8	BaO				
2	Y_2O_3				
1	O_2				

If the equation is balanced, the indicator in the left bottom corner of the window reports "**Balance_Ok**". If the indicator is red and reports "Balance IS NOT FULL", click it to see reasons in the balance window. If the Autocalculation of coefficients is turned on, the indicator in the right bottom corner of the window reports about the status of coefficients calculation - "One solution ", "Several solutions" or "No solution". In the last case, click the indicator to see reasons in the window of invalid solution reasons.

It is often necessary to know masses of reagents and products. For this purpose input the mass of one reagent or product into corresponding field. This field will yellow. The other masses will be calculated automatically. If you input "100" as the product mass in our example table, the former will look as follows

Coeff.	Reagents	Masses	Coeff.	Products	Masses
12	CuO	35.82085	4	$YBa_2Cu_3O_7$	100
8	BaO	46.03058			
2	Y_2O_3	16.94777			
1	O_2	1.20081			

Output can be sent to a printer or to another WINDOWS program. UrChemCalc saves the last equation for use at a later time (files CONFIG.*) - you can continue your work from this point at the next time.

Attention! Calculation results are valid only if the chemical compound database and the chemical element database are valid.

Balance window

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This window is opened by clicking the balance indicator in the main window in the case of invalid balance. The window contain the information about balance on all chemical elements in the reaction. In the bottom part of window are placed following buttons:

Ok - close the balance window, return to the main window;

Help - call UrChemCalc Help (this page).

The window of invalid solution reasons

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This window is opened by clicking the solution status indicator in the main window if the valid solution of the problem of automatic calculation of the reaction equation coefficients is absent. The window contains the information about the probable reasons of this error. In the bottom part of window the following buttons are placed:

Ok - close the window, return to main window;

Help - call UrChemCalc Help (this page).

Solution wizard

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The wizard solves the problem of composing the records of chemical compound database, related to the binary mixtures (liquid or solid solutions, compounds with admixtures, etc.). It transfers from the different forms of concentration to molar fractions and put it into current database record.

Click the button  in the chemical compound database window. Be care - the wizard will edit the current record! If the solution must be in a new record, dont forget to click the button **Insert** in order to make an empty place!

In top part of the wizard window two fields - *Solute* and *Solvent* are placed. You can choice it values from the list of chemical compounds in the database. There is the field below these fields, which has the own list of values contained the available methods of concentration description. Choice the method you need and input the required numbers.

In the bottom part of window the following buttons are placed:

Ok - Close the wizard window with transferring of the result into the current record of chemical compound database. The program checks values in all fields in this process;
Cancel - Close the wizard window without transferring of the result;
Help - Call UrChemCalc Help (this page).

I recommend you the solution wizard as the most accurate method of writing the records with solutions, which concentration is known in form differ the molar fractions. If you don't like the formulae concocted by the wizard, try to use the service of dividing all coefficients by one of them or any another. You can do it by double clicking the coefficient field. This convenient method keeps the accuracy of proportions between elements.

How can I register?

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Ural Chemical Calculator can be registered via following steps:

- fill in the registration form and send it to **lakhtin@hotmail.com**
- replay email will contain the total registration fee (about $30 per copy) and payment method;
- the registration fee is paid as outlined in the email;
- next email to you will contain your unique registration number(s) and the detailed instruction after which your copy(ies) becomes the registered.

The registered copy of UrChemCalc has output options. Program developer answers questions of registered users via E-mail. Unregistered copy may be used for only 30 days (see License Agreement).

Automatic calculation of the equation coefficients

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This option may be turned on by the switch near the center of the bottom part in the main window. If the switch is turned on  , UrChemCalc automatically calculates coefficients of reaction equation (except fixed coefficients). Special indicator in the right bottom corner of main window reflects the status of the calculation:

- "One solution" - the calculation is successful, the result coefficients are placed into corresponding fields;
- "Several solutions" - the calculation is successful, but the result is ambiguous. One available set of coefficients is placed into corresponding fields;
- "No solution" - the material balance cannot be achieved under all conditions. In this case click the indicator to find reasons in the window of invalid solution reasons.

Examples:

$Cu + CuO = Cu_2O$ - One solution

$3Cu + O_2 = CuO + Cu_2O$ - Several solutions

$CuO + BaO = Cu + Ba$ - No solution

Fixed coefficients are invariable in the automatic calculation process.

Choice of the compound name from the list

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The list of compound names appears after clicking on any field of compound name in the main window and fields *Solvate* and *Solvent* in the window of solution wizard. The list are formed by the alphabet sorted records of the chemical compound database and appended (in main window only) by empty line and reserved phrase "New compound". The list is scrollable. Key search is available by typing a few first symbols. Key is visible, <Backspace> and <Escape> erased the key partially and exactly.

The choice of reserved phrase "New compound" activates the edit window for a new database record. The choice of empty line (at the top of list) may be used to clean the compound name field in main window. Click the menu item **Reset** to clear all fields.

Language

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Click the menu item **Language** in the main window to see the list of available languages used by this version of UrChemCalc for user interface. Click the language to set it. To have a success a few national fonts must be preinstalled in your system (there is not any problem, if you use the localized WINDOWS version).

UrChemCalc Help is not the same for all languages. It is most complete in Russian, because Russian is my favorite language. Besides, the texts in other languages may contain many mistakes. I am very sorry, but the situation is as it is.

Fixed coefficients

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The fixed coefficients in the main window are shaded with the aqua background color, in contrary to the white color of free coefficients. Use the popup menu of coefficient fields to fix or free it. The manual editing of these fields automatically fixes coefficients.

If the switch Autocalculation of coefficients is turned on, the free coefficients are the automatic calculation results (if a solution exist). The fixed coefficients are constant in the calculation process.

If the switch Autocalculation of coefficients is turned off, there are not any differences between the fixed and free coefficients, except its colors.