MineralMatch

Software Tools for Mineral Identifcation

User manual

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Content

Introduction

MINERALMATCH is software intended to assist in the determination of the mineralogy of analyzed phases. The program uses the input compositional data from a quantitative analysis to find the best match from an extensive database containing thousands of minerals.

Identifying a mineral can be a complex task, and this program should be viewed as a tool in that identification process, not as the final word. It is still up to the user to make the final decision.

As students of mineralogy know, different mineral species can have both identical compositions (polymorphs) and similar or overlapping compositional regions. This program uses the distance in compositional space to identify the nearest mineral match. However, not all elements in a mineral have the same importance in differentiating one mineral from another. Consider the pyroxene mineral system (Fig. 1).

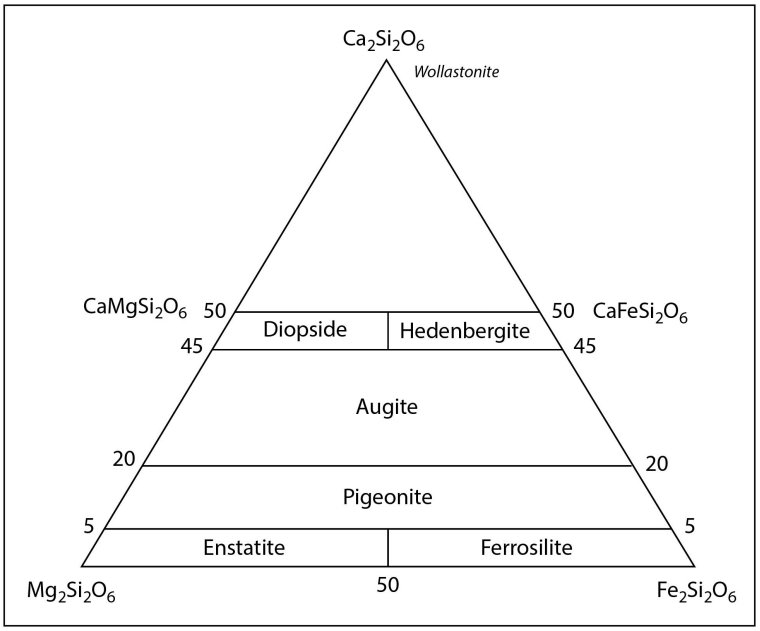


Figure 1. Mineral relationships in the pyroxene ternary (after Deer, et al, 1992).

The ratio of Fe/Mg will differentiate enstatite from ferrosilite, and diopside from hedenbergite, but not augite from pigeonite. Both of the later two minerals have complete solid solution in Fe and Mg, and are differentiated based on their Ca content. Therefore, using the total compositional distance of all the elements may lead to an erroneous match. For example, assume one has an analysis of an unknown, which actually has a pigeonite composition (dot-circle, Fig. 2) and compares it with a set of analyses from the database (red dots, Fig.2). In the example in Figure 2, the unknown would be closest in compositional space to the augite analysis "A". However, identifying the unknown analysis as an augite would be incorrect since the unknown analysis has too little Ca to be classified as such.

This problem can be corrected by combining the Fe and Mg into a single component before searching for a match. If (Fe+Mg) is considered as a single component, as opposed to two components, then the closest database analysis to this unknown would either be analysis C or D. Both would identify the unknown correctly as a pigeonite.

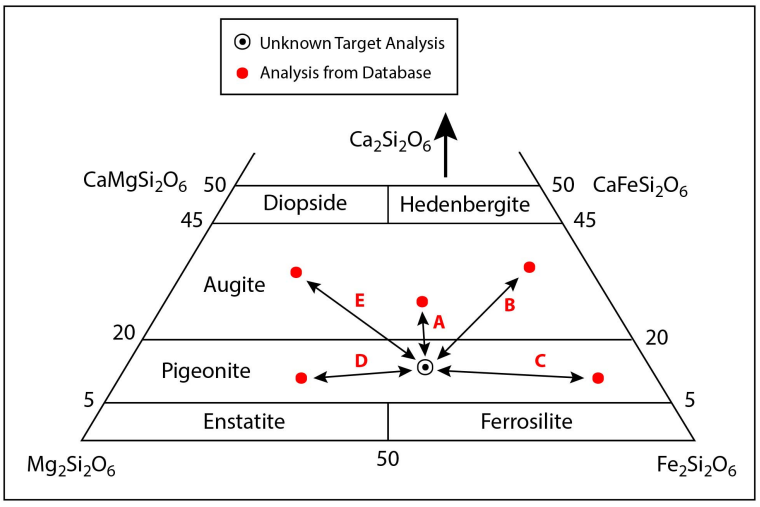


Figure 2. Pyroxene system with an example of an erroneous mineral match resulting from considering all elements to be of equal importance.

The MINERALMATCH program provides the user with tools for analyzing their varied compositional data sets. These include:

- **Adding missing elements.** Often H_2O or CO_2 have not been included in an analysis. However, they may constitute an important component within the mineral. If the user suspects their analysis is missing such a component, one can add those elements as either fixed values or by difference, before searching the database.
- **Ignore selected elements.** Some elements are difficult (B, Be, C, N) or impossible (H, Li) to analyze for. For this reason a user may choose the option to ignore those elements from both the target analysis and the database, allowing the nearest neighbor calculations to be restricted only to those elements with a high analytical confidence.
- **Group all Rare Earth Elements**. The ratio of the rare earth elements (REEs) might be useful in determining the specific mineral species, but rarely in determining the mineral group. Combining the REEs together might be helpful in the preliminary searches.
- **Ignore minor elements.** Typically, minor elements have little or no importance when categorizing mineral species. However, cumulatively they may affect the quality of the match. A threshold can be set that will allow elements to be ignored if they fall below a specified value set by the user.
- **Allocating elements to mineral sites**. Many minerals allow for element substitutions, which do not effect the categorization of the mineral species, or at least the mineral group. Users can specify which elements should be considered as occupying a single site. Those elements will then be combined during the search process.
- **Calculate site occupancies.** Once the elements have been allocated to sites and the anion normalization factor has been defined, a worksheet will calculate the site occupancies (number of atoms per site per formula oxygen). This is another way to assist the user in selecting the most likely matching mineral.

- **Mineral formulas**. MINERALMATCH contains nearly 5,000 mineral formulas that can be searched by mineral name or mineral group name.
- **Search by compositional range.** Besides searching for a mineral match based on a specific analysis, a search can also be run based on user-selected elemental ranges.
- **Search by mineral name.** Users can search for a mineral analysis in the database using the mineral name or group name.
- **User libraries**. A user can define any number of user libraries to be used for later searching - a more selective, customized substitute for the built-in Master Library.
- **Batch searches.** Once a User Library has been defined that contains all of the likely minerals involved in a project, thousands of analyses can be cataloged by mineral name using a batch process.

Nomenclature

MINERALMATCH uses the term "Target" for the unknown composition provided by the user to be identified.

The term "Match" is used for the minerals found in the program's database, which have been calculated to be closest in composition to the Target.

The main window has two display regions (Fig. 3), the upper "Main Display" and the lower "Individual Tab Displays".

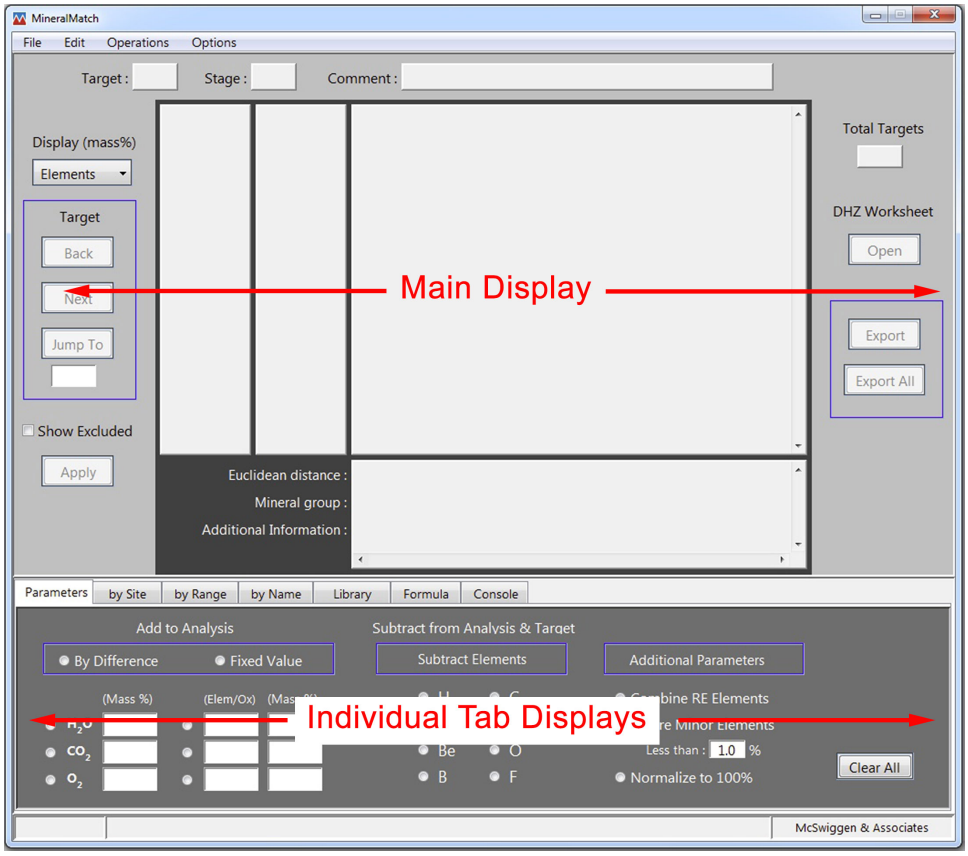


Figure 3. Layout of the displays in the program's main window.

Input Analyses

There are three methods for data entry users can choose from in the software, (1) read JEOL Qnt data that was collected on a JEOL EPMA, (2) read data stored in a text file, and (3) manually enter the data directly into the program.

Import JEOL Qnt Data

MINERALMATCH can read the JEOL Quantitative Analysis data directly as long as (1) the data was collected on a JEOL JXA-8230, JXA-8530F, JXA-8530F Plus, JXA-iSP100, or JXA-iHP200F, and (2) the data has been previously opened with the JEOL Summary program. The JEOL Summary program creates the files used by the MINERALMATCH program.

To import the JEOL Qnt data, go to the File >> Open >> JEOL Qnt menu item. The window below will open (Fig. 4).

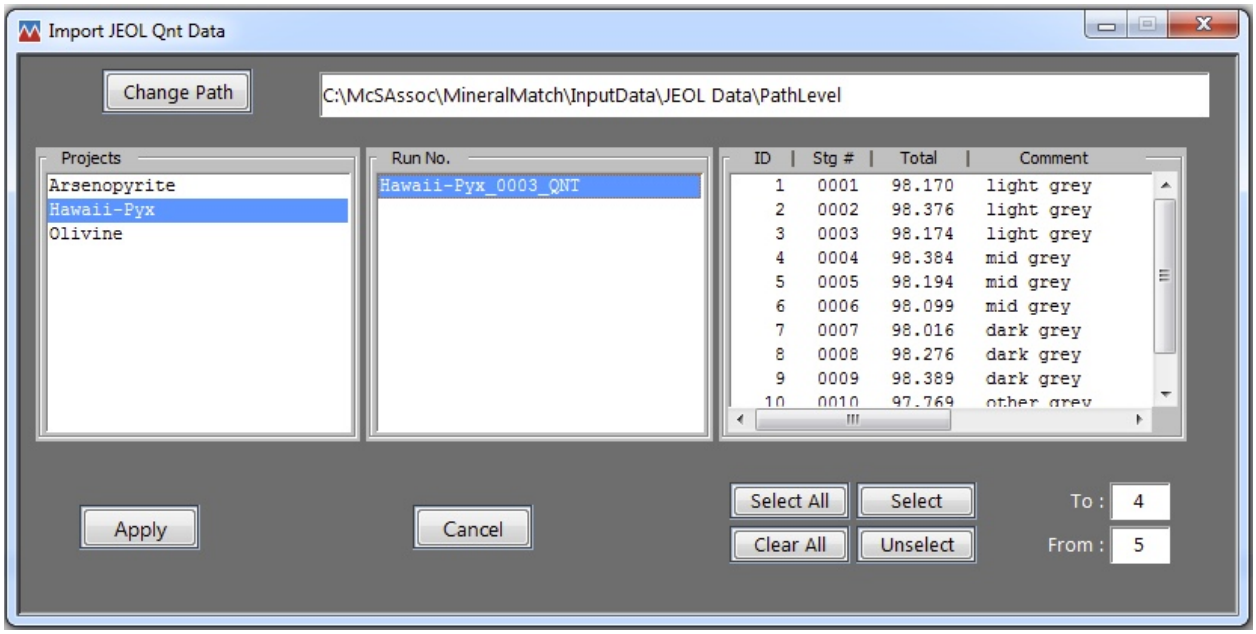


Figure 4. Window for importing JEOL Qnt data.

If the "Path" is pointing to a directory containing JEOL Projects, which in turn contain JEOL quantitative data, MINERALMATCH will recognize that fact and it will display all of those Projects in the Project List on the left side of the window. It will not display any directories that do not contain quantitative data in a recognizable JEOL file format. If the Project List is empty, then the Path must be changed to a suitable directory containing the desired quantitative data. Click on the "Change Path" button. This will open a standard file chooser window. Select the desired directory. Be sure the directory **above** the desired Project is selected. If a directory that is either higher or lower in the file structure is selected, the quantitative data will not be recognizable and nothing will be displayed in the "Import JEOL Qnt Data" window.

Once the proper Path has been selected, all the Project directories that contain JEOL Qnt data will be displayed in the Project List. By selecting one of these Projects, the list of Qnt Runs within that Project will be displayed in the Run List in the middle of the window. By selecting one of the Runs, all of the individual analysis points that were collected as part of that Run will be displayed in the Stage List on the right.

One or more points can be selected from the Stage List. At a minimum, one point must be selected. An individual analysis can be selected using a mouse click, and a group of points can be selected using the combination of <shift><mouse click>.

Groups of points that are not continuous can be selected using the provided buttons: "Select All", "Clear All", "Select" and "Unselect".

- **Select All** - will automatically select all of the analytical points in the list.
- **Clear All** - will deselect all of the points in the list.
- **Select** - will only select those points falling within the numerical range of those values entered in the "To" and "From" boxes.

- **Unselect** - will deselect those points falling within the numerical range of those values entered in the "To" and "From" boxes.

For example, if one would like to select two groups of analyses, one could enter the highest and lowest index values of the two groups in the "To" and "From" boxes. Clicking on the "Select" button will select the entire range of points. Then enter the sub-range of values within the larger range that are to be excluded, and click on the "Unselect" button. Now two groups of analysis points are selected that will be loaded into the MINERALMATCH program (Fig. 5) once the Apply button has been selected.

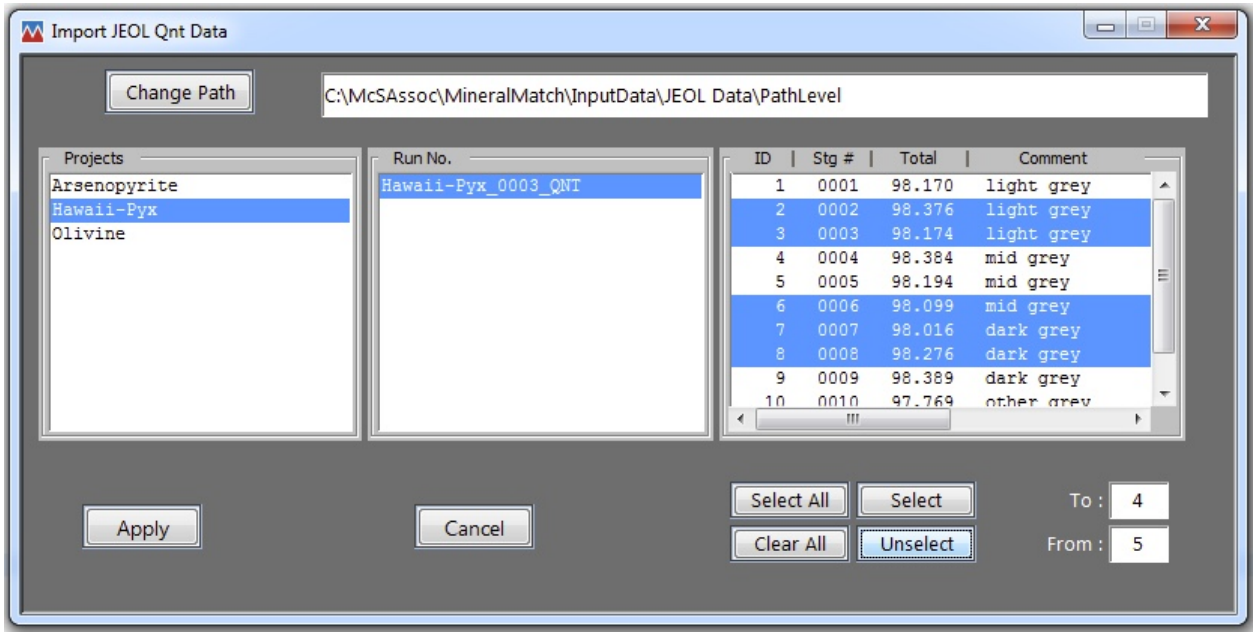


Figure 5. *Window for importing JEOL Qnt data with multiple ranges of analytical points selected using the "Select" and "Unselect" buttons.*

Once the desired analytical points have been imported into the MINERALMATCH program, the program will load the first "Target" analysis into the Main Display (Fig. 6; label #1). The JEOL stage number is listed at the top (label #2), as is the original analytical comment (label #3).

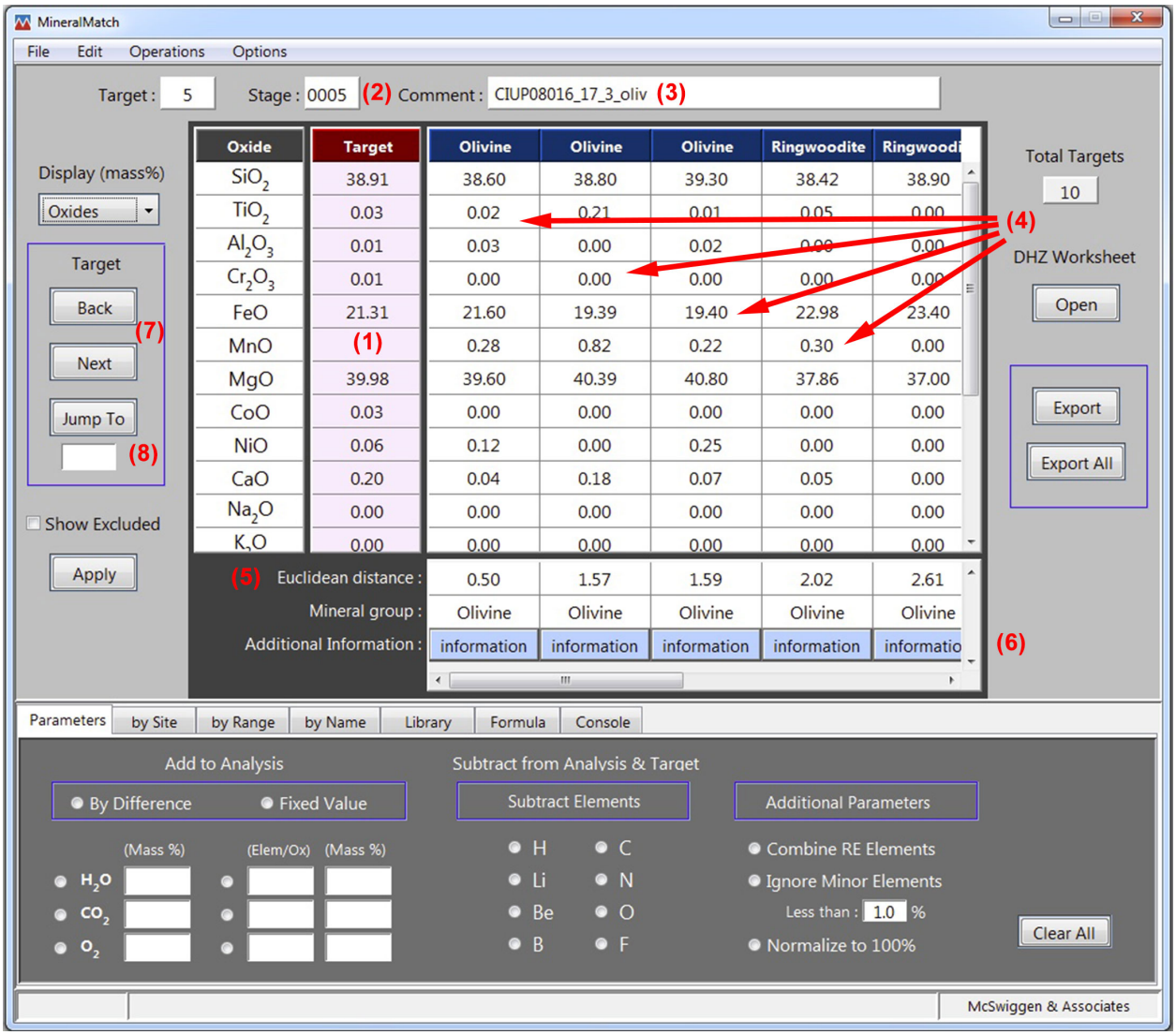


Figure 6. Main display after a Target analysis has been loaded and a search for the best Match has been run.

The MINERALMATCH program automatically calculates the compositional distance between the Target analysis and every analysis contained in the selected mineral database. It then displays the 10 closest mineral analyses in the Match columns (label #4). The compositional distances are listed in the lower table (label #5), identified as the Euclidean distance. The lower the value, the closer the Target mineral is in composition to the Match mineral.

The "information" button at the bottom of each Match analysis (label #6) contains additional information about the analysis, including the published

source (Fig. 7). The Comment box allows the user to add any additional information to the mineral for future reference. The "Exclude" button at the bottom of the window allows the user to exclude this analysis from all future searches. This is useful for minerals the user knows will never be encountered in their work, for example, high-pressure, polymorphs of common minerals. All of the mineral analyses that have been marked as "Excluded" can later be displayed as part of a search by clicking on the "Show Excluded" check box on the Main Display (Fig. 8, left side). Those previously excluded analyses will show up with a light-gray highlight in the Match columns.

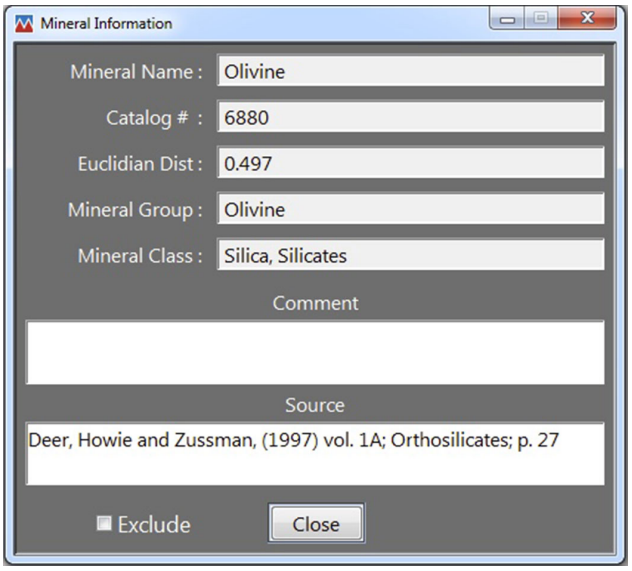


Figure 7. Mineral Information window displayed by selecting the "information" button.

Finally the "Next" and "Back" buttons are used to step through the list of Target analyses that were imported into the program (Fig. 6; label #7). Each time one of the two buttons is selected, a new Target is displayed and the full database search is run. To avoid stepping through a long list of Target analyses, a particular Target can be displayed using the "Jump To" button and corresponding text box (Fig. 6; label 8).

By default the data is initially displayed in the form of element mass percent. However, if the analysis is that of an oxide mineral, by changing the "Display

(mass%)" drop-down menu to display "Oxides" (Fig. 8, label #1), the Target and Match analyses will be recalculated into the oxide form. The mass percent of each oxide is calculated based on the stoichiometry of the valance of the specific cation. It is ***not*** calculated from the reported amount of oxygen in the analysis. Therefore the user must use this feature with discretion. It is up to the user to know when it is appropriate to display the results in their elemental or in their oxide form.

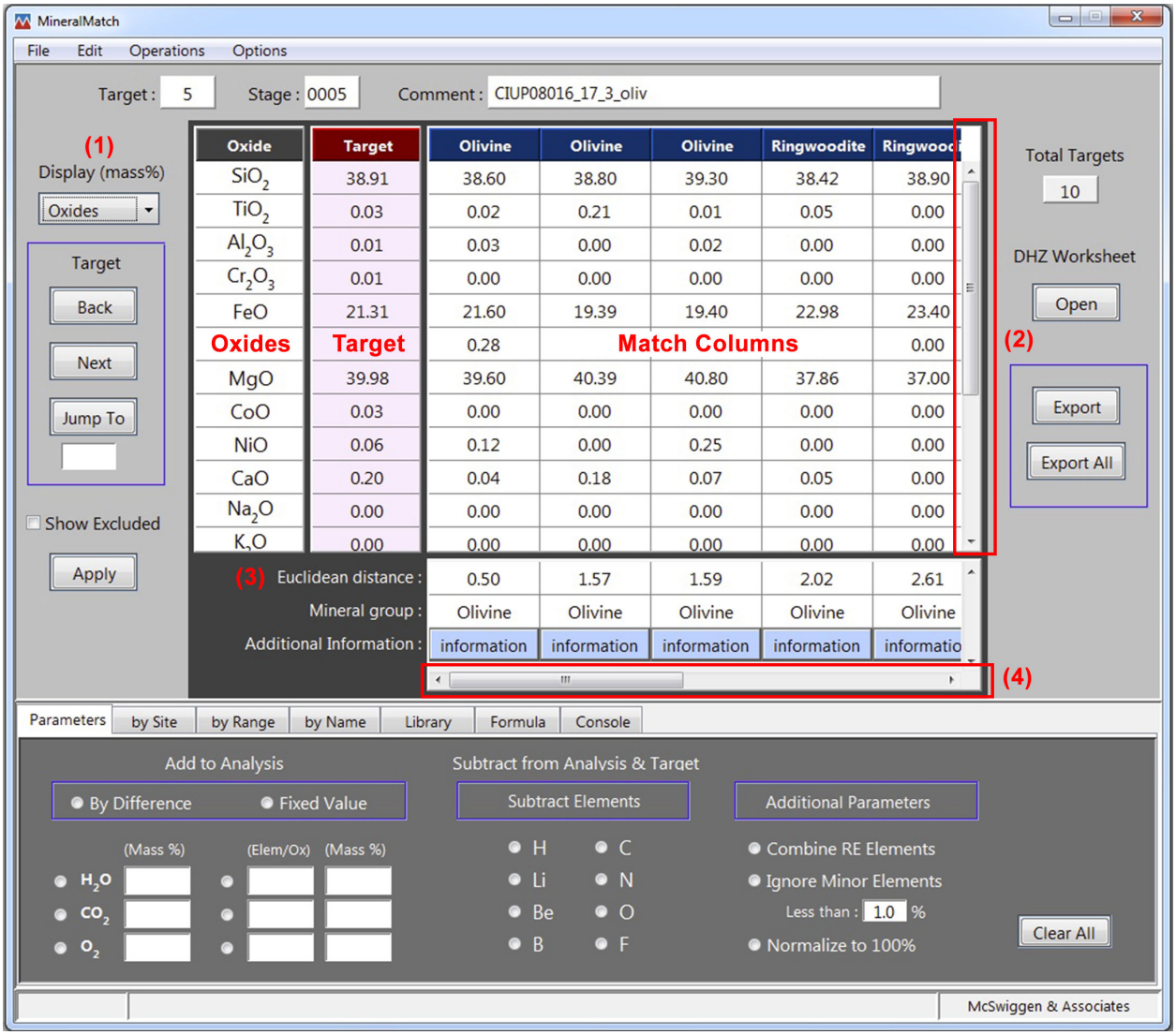


Figure 8. Main display with the analyses converted to an oxide form.

The Main Display contains four tables (Fig. 8). The left most one contains the element or oxide list. The next table to the right contains the Target analysis, and the right multi-column table contains the Match analyses. There is only one vertical scroll bar that controls the vertical motion of all of these tables (Fig. 8, label #2).

Below the Match table is a fourth table containing the Euclidean distance value calculated between that particular Match mineral and the Target analysis (Fig. 8, label #3). The lower the value the closer the match. A value of zero means the two compositions are identical. At the bottom of this table is the horizontal scroll bar (Fig. 8, label #4) that controls the horizontal motion of both this table and the Match table above it. This allows the two tables to always be in sync while looking at the total list of minerals in the Match table.

Import Data from Text Files

Compositional data can be imported into MINERALMATCH from a text file stored in a variety of formats. MINERALMATCH does not force the user to use a predefined data arrangement. The data can be arranged either by column or row, and can be separated by tabs, commas, or by white space.

To open a text file, select the menu item, *File >> Open >> Text*. This will open a standard file chooser. Select the text file of interest by name. This will open the Import Text File window (Fig. 9).

The content of the file will be displayed in the window's listing ("File Content" display in the center of the window). On the left side of the file listing, MINERALMATCH includes a sequential numbering of each line. This numbering is separated from the actual file data by two vertical lines "||". The line numbering has been added to make it easier for the user to discern the number of any header or footer lines.

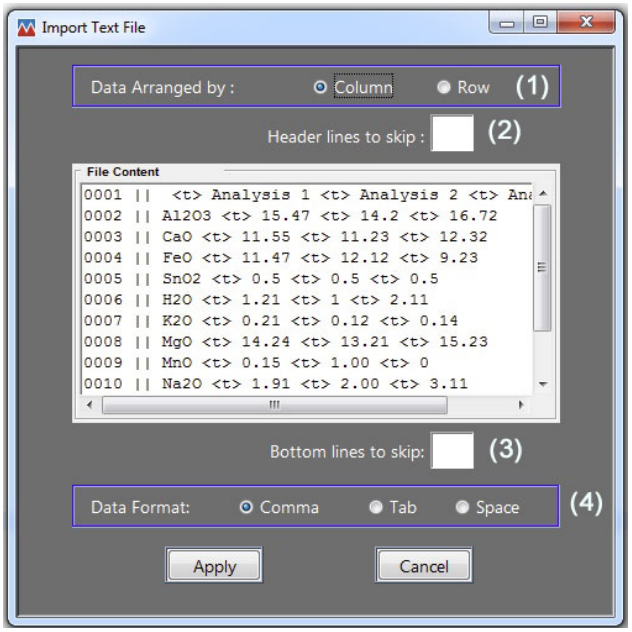


Figure 9. Import Text File window.

Given that the data may be arranged in either a column or row format, the user must select that which applies to their specific file (Fig. 9, label #1). Column data is arranged so that each analysis occupies only one column, and row-formatted data occupies only one row per analysis. This can be determined by inspecting the file content.

If there are header lines at the top of the file not needed as part of the data set, they can be removed before importing the file by entering the number of those lines (Fig. 9, label #2). Lines at the bottom of the file that are not part of the analyses should also be removed (Fig. 9, label #3).

Tabs, commas, or space can be used to separate the data items in the text files (Fig. 9, label #4). Tab markers in the data set will be displayed as "< t >". If white space is to be used to separate the data, make sure that there are no spaces used in the analysis labels. This would result in the label being separated into different columns. The recommendation would be to replace the spaces within a label with an underscore ("_"). Using tabs or commas as separators will lead to fewer potential problems. These are recommended over white space.

Once the parameters above have been set, the "Apply" button will cause the file contents to be parsed and displayed into one of two windows "Edit Import Table - Column Data" or "Edit Import Table - Row Data" (Fig. 10). If the wrong parameters were initially selected, simply close the window that has opened using the "Cancel" button and try again.

These Edit Import Table windows are used to further edit the text data before the final import. At a minimum, MINERALMATCH needs to know which column or row contains the element list and the analysis labels.

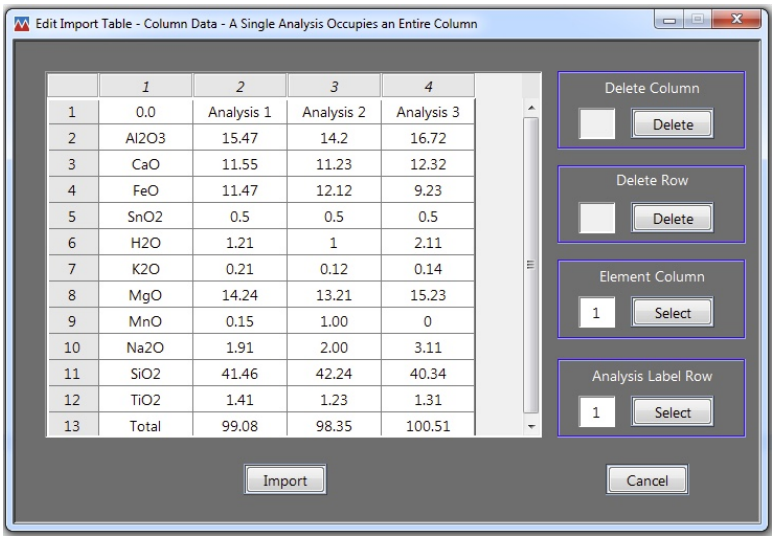


Figure 10. Edit Import Table - Column Data window before the element column or analysis label row has been selected.

For column-arranged data, typically the first column contains the element list and the first row contains the analysis labels. Therefore, the Element Column box and the Analysis Label Row box have a "1" entered in them by default. These values can be changed if other columns and rows contain those data items. Once the Element Column "Select" button is selected, the element column will be highlighted in pink (Fig. 11).

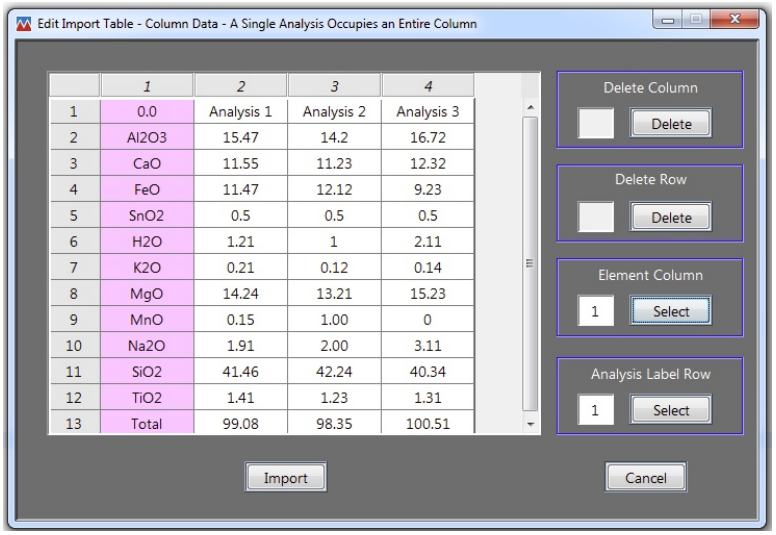


Figure 11. Edit Import Table - Column Data window with the element column identified.

Similarly, once the Analysis Label Row "Select" button has been selected, the analysis label row will be highlighted in yellow (Fig. 12). This highlighting is displayed to allow the user to be confident that the program has identified the proper column and row.

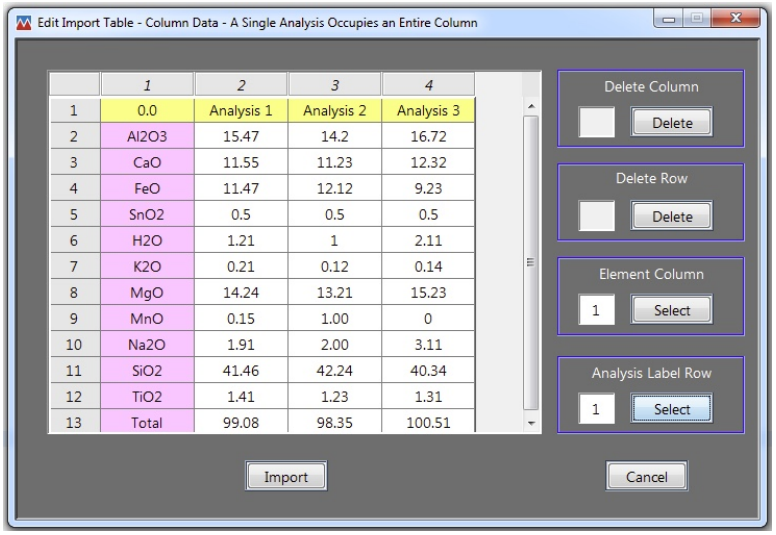


Figure 12. Edit Import Table - Column Data window with both the element column and the analysis label row identified.

Some data files contain more extraneous information that is not part of the analyses and which cannot be excluded by eliminating header lines or lines at

the bottom of the file (Fig. 13). These extra columns or rows MUST be removed before the file is imported. No data should be imported from the text file that is not (1) the list of elements, (2) one set of labels for the analyses, and (3) the compositional data itself. All other extraneous rows or columns of information must be deleted before attempting to import. Any other labels or summary data will result in failure of the file import.

If a column needs to be deleted, simply select a few of the table cells within that column. The software will identify which column was selected, and enter that column number into the Delete Column box (Fig. 13). To remove the column, click on the associated Delete button.

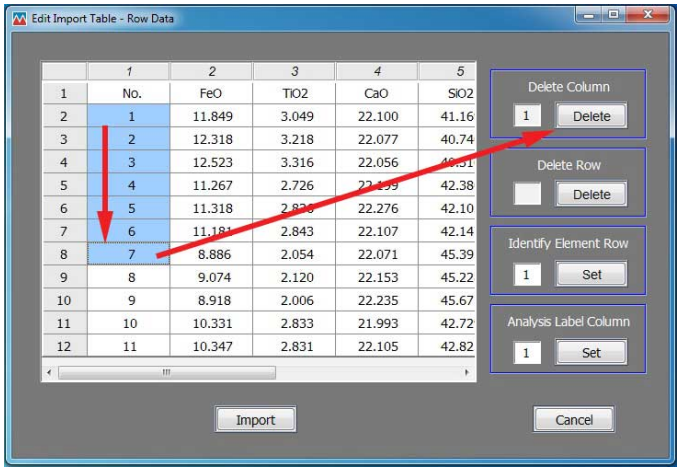


Figure 13. Edit Import Table - Row Data window with a column selected for deletion.

To delete a row, the same procedure can be followed. Click and drag along one row. The software will identify the row and will enter that row value into the Delete Row box. Click on the associated Delete button to remove it.

Input an Individual Analysis Manually

The MINERALMATCH program allows the user to enter a Target analysis directly into the program, bypassing the need to access the data through another file. Going to the *Operations >> Single Pt* menu item will open up the Enter Single Point Analysis window (Fig. 14).

Before entering any data, first determine whether the analytical data is in mass percent of the oxide or the element. The data must be in the form of mass percent, but can be in either the elemental or oxide forms. Before entering any data, select either the Element or Oxide button (Fig. 14, label #1). If one has started to enter the data in the opposite format from that which was selected, **all** of the previously entered data must be deleted before switching to the other format.

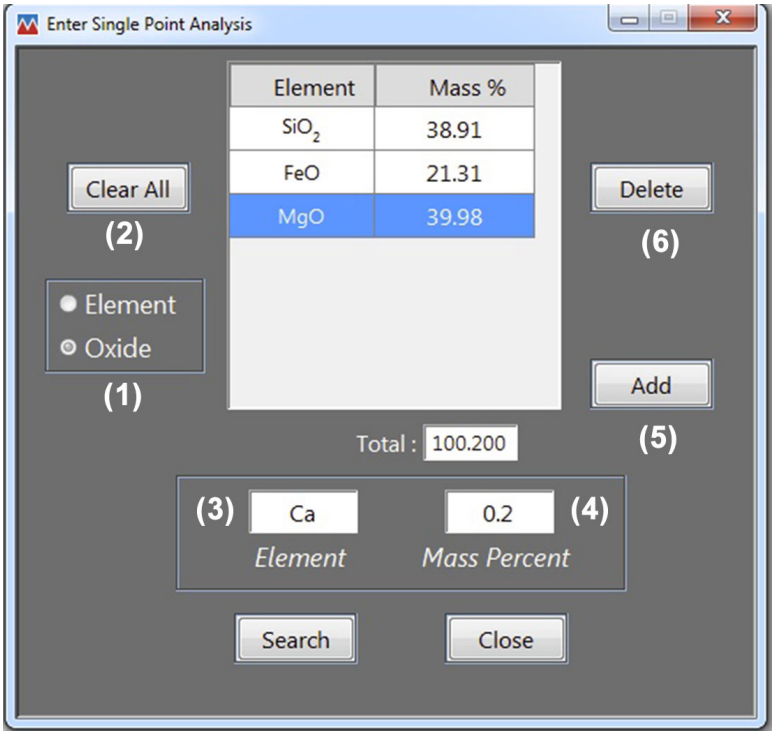


Figure 14. Enter Single Point Analysis window.

This can be done using the Clear All button (Fig. 14, label #2). Now start re-entering the data. Type the element symbol into the Element box (Fig. 14, label #3). Do not enter the oxide formula, even if the Oxide form has been selected for the data being entered. The software will determine the oxide formula based on the element symbol and the list of preferred oxide types (see **Changing Options**, page 46). Now enter the mass percent (Fig. 14, label #4) of either the element or oxide, depending on whichever is selected (Fig. 14, label #1), and then click on the Add button to add this data to the database (Fig. 14, label #5).

If a mistake has been made while entering the data, the element and its data can be deleted by selecting the incorrect element's row and then click on the Delete button (Fig. 14, label #6).

Once the data has been entered, click on the Search button (Fig. 14). This will automatically search the entire database for the closest matching minerals, will display the entered Target composition, and will display the closest matches in the Main Display.

Advanced Searches

As soon as a compositional analysis has been read into the program, a search is automatically initiated to find the minerals in the database that are closest in composition. However, as previously mentioned, there may be situations in which other parameters should also be considered in order to constrain the search and thereby help to identify better matches.

"Parameters" Tab

The Parameters Tab display (Fig. 15) at the bottom of the main window allows the user to add, subtract, and combine elements in Target and Match analyses. The objective is to correct for deficiencies in the original analysis or to remove the influence of elements that are not important in the mineral identification.

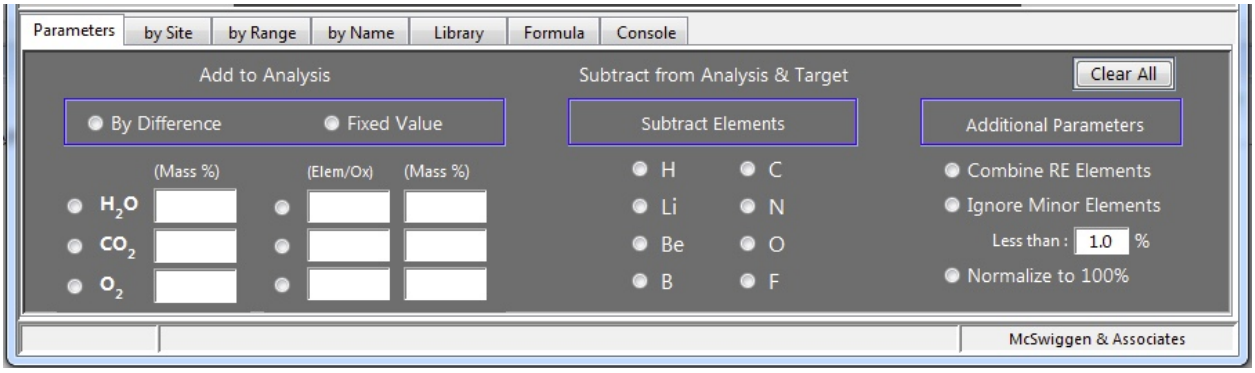


Figure 15. Parameters Tab used to add, subtract, or combine elements before searching.

The left side of the display in Figure 15 is used to add elements to the analysis. Typically, the most common addition(s) would be water, CO_2, or extra oxygen. These would be added back to the analysis in cases where the user did not analyze for them in the original analysis, but felt that one or more of them might be in the mineral. These might be suspected because of the low analysis total, the basic composition of the mineral, or a combination of the two.

As an example, if an oxide mineral was analyzed and it had a low analytical total, a high abundance of Fe, and the Fe was analyzed as FeO in the original analysis; this might cause one to consider that some of that Fe was in the form of Fe_2O_3. If this were true, then there would be O_2 deficiency in the analysis. This could be corrected for by adding in extra oxygen back into the analysis before running the search.

The oxygen could be entered as a Fixed Value or "By Difference". If the oxygen was going to be added by difference, then the "By Difference" button would be selected, as well as the "O_2" button. Nothing else is required.

If the oxygen was going to be added as a fixed value, then the "Fixed Value" button would need to be selected, as well as the "O_2" button. In addition, the amount of O_2 that was to be added would need to be entered into the O_2 box, as shown in Figure 16.

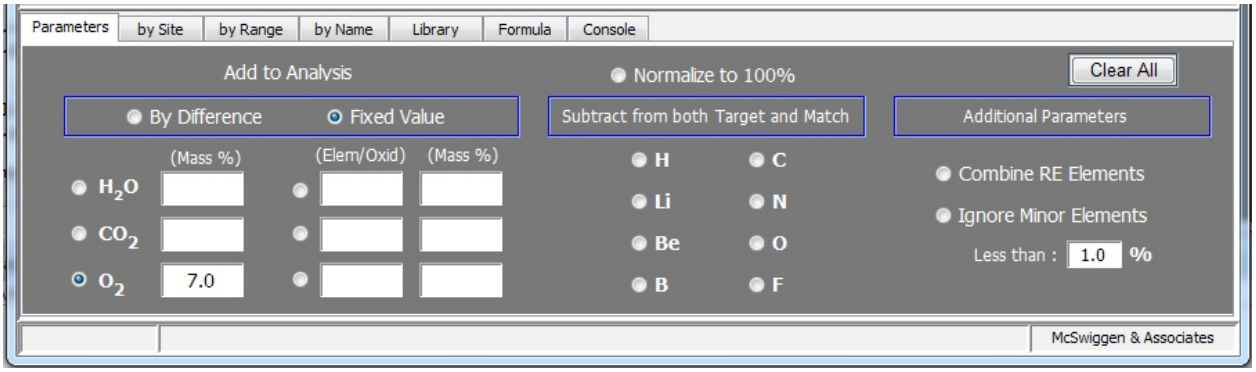


Figure 16. Parameters Tab with additional O_2 being added as a fixed value.

Similar procedures will work for both H_2O and CO_2. Space is also provided for up to three other elements or oxides. If another element or oxide is to be added, enter its name in one of the boxes under the "(Elem/Oxid)" heading. Both the element symbols and oxide formulas are valid entries. The program recognizes both. Check the button next to the name. If the component is to be added by difference, leave the "(Mass %)" box empty. If it is to be added using a fixed, value enter the amount in the "(Mass %)" box (Fig. 17).

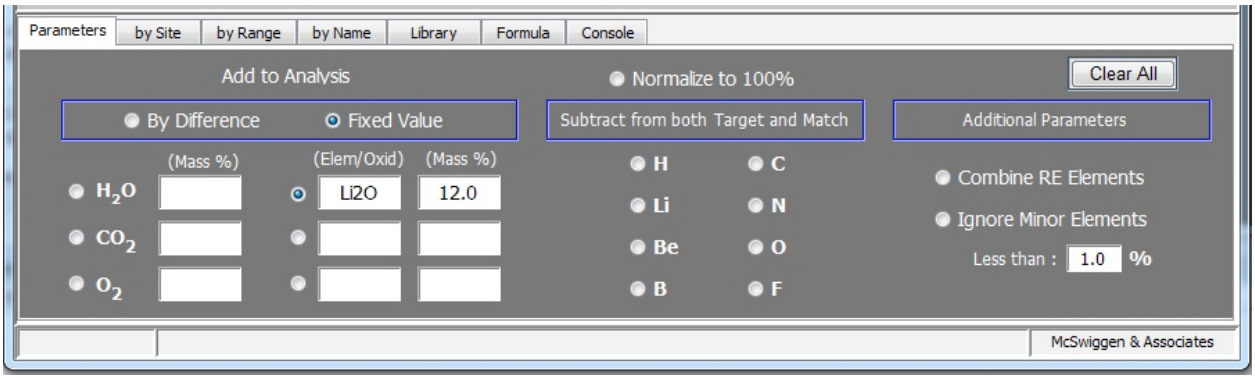


Figure 17. Parameters Tab with LiO_2 being added to the analyses as a fixed amount.

A new search, or the implementation of any new search parameters, will only occur when the "Apply" button is selected in the Main Display (Fig. 18, #1).

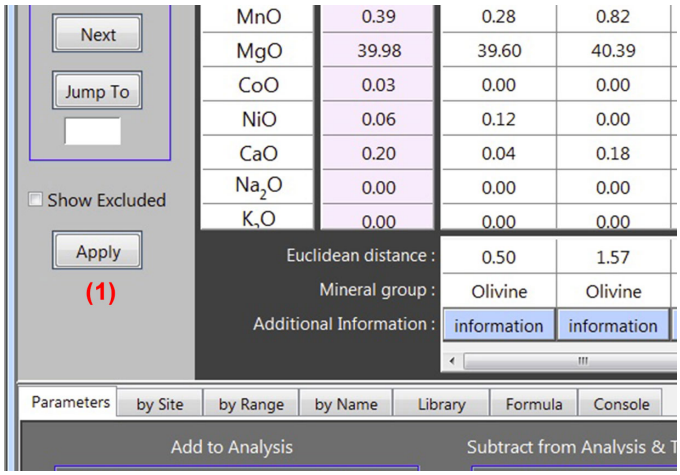


Figure 18. Lower corner of the Main Display showing the location of the Apply button, which is required to re-run a search using the advanced search parameters in the Parameters and by Site Tabs.

In the center part of the Parameters Tab, the user can subtract the elements from both the Target and Match analyses, and on the right are additional parameters for controlling the method by which the analyses are compared (Fig. 19).

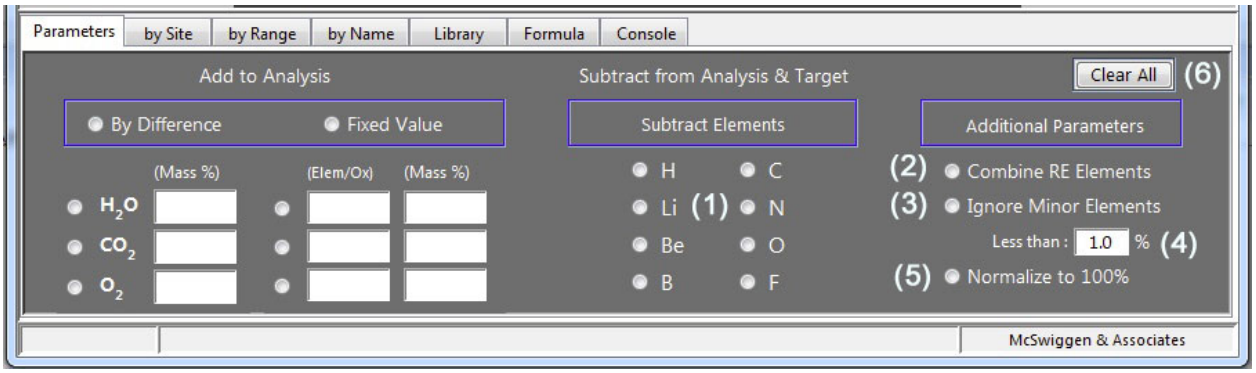


Figure 19. Parameters Tab highlighting the controls for normalizing the Target analysis and for subtracting elements from both the Target and Match.

Given the challenges involved in analyzing light elements, there might be situations where one might get better results in the match-searches if those elements were excluded from the search. By selecting those elements in the Parameters Tab (Fig. 19, label #1), the element will be removed from both the Target and the Match database before running the search. This would allow only for those elements in which the user had high confidence in their accuracy to be used in the search.

Rare earth elements add a complexity of their own to the searches. The specific the rare earth elements (REE) ratios are commonly incidental when it comes to identifying the REE mineral group to which the mineral belongs. Therefore, at least as part of the preliminary search, it might be advisable to combine all of the rare earth elements into a single total REE mass percent value (Fig. 19, label #2). This eliminates the distraction stemming from, for example, whether the Cerium is the dominant REE or the Lanthanum.

Likewise, minor elements can be a distraction when trying to identify the proper mineral species from an analysis. Typically the minor elements are not the deciding criteria, but collectively they could divert a match calculation away from the true match mineral. For this reason, the option is provided to remove minor elements from both the Target and Match (Fig. 19, label #3). The user sets their desired threshold (Fig. 19, label #4). An element concentration below the value entered will result in that element being ignored.

The Target and Match data can also be normalized. If the user concludes that a low total in the Target analysis is due to an error in the analysis that generally affects all elements equally, then it might be advisable to normalize the data before running the match search (Fig. 19, label #5). Examples of where this might be helpful include a situation where the beam current was not properly corrected for, when working with ultra thin samples, or when the sample had a carbon coating that was inappropriately either too thick or too thin.

The Clear button will remove all of the data entered into this tab by the user (Fig. 19, label #6).

"by Site" Tab

Defining a mineral based solely on its composition can be complicated. Each mineral has a nominal composition that can be derived from its formula. However, the actual composition of a mineral can vary greatly. The amount of variability is defined only in the most common minerals. However, the formulas can give considerable guidance.

The formula for the plagioclase mineral, albite, is $NaAlSi_3O_8$. At the other end of the plagioclase series is anorthite with the formula, $CaAl_2Si_2O_8$. There is complete solid solution between these two end-members. Therefore a formula for the plagioclase series could be defined as $(Na,Ca)Al(Al,Si)Si_2O_8$.

Because of the solid solution in this mineral series, the ratio of Na/Ca atoms is immaterial within the plagioclase series, as long as the total atoms of (Na + Ca) = 1, after normalization to 8 oxygen. Therefore using both Ca and Na as separate components, when searching for a mineral match, might not be the best strategy in this situation. It might be better to combine them into a single component. The "by Site" Tab of the MINERALMATCH program allows the user to define which elements should be grouped together into sites.

This process of grouping the elements can be used for both searching for a mineral match and later used to evaluate to what degree the Target analysis fits the mineral formula of the matched mineral (DHZ Worksheet). Figure 20 shows the layout of the "by Site" Tab.

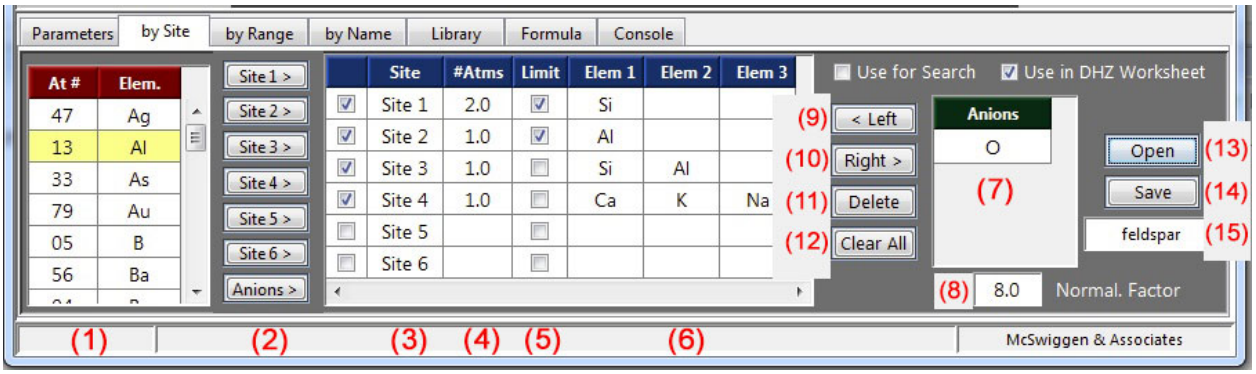


Figure 20. Layout of the "by Site" Tab.

On the left-hand side of the tab display is the list of the elements in the periodic table (Fig. 20, label #1). Any of those elements can be added to any particular site defined by the user. By default, the elements are listed alphabetically. However, the user can re-sort the element list to be either numerically sorted by atomic number or alphabetically sorted by element symbol. To switch back and forth, simply click on the "At#" or "Elem." header.

To add an element to a particular site, select the element (it will be highlighted in blue), and then click on the specific site button (label #2) for the site the element should be included with (label #3). The element will now appear in the element list for that site (label #6).

If an element in the periodic table list is highlighted in yellow, this means that the element has already been added to one of the sites. An element can be added to more than one site, but not multiple times within the same site.

The "#Atms" column of the site table (label #4) allows the user to specify the maximum number of atoms that the site can hold. This has no bearing on the

mineral match searching. However, it does affect how the elements are distributed in the DHZ Worksheet (to be discussed later).

In this example (Fig. 20), Si has been entered into site #1 and the maximum site occupancy has been set to 2. Al has been added to site #2 with a maximum occupancy of 1. Si and Al have then been added again into site #3, but without selecting the "Limit" check box. As a result, if there are more than 2 atoms of Si, site #1 will be filled up and the remaining Si will be added to site #3. Likewise, if there is more than one atom of Al, site #2 will be filled and the remaining Al will be added to site #3. Since the Limit check box has not been selected for site #3, all additional Si and Al will be added there, regardless of how many total atoms this comes to.

Ca, K, and Na are all allocated to site #4, with no maximum site occupancy given. Therefore all of the Ca, K, and Na will be entered into this single site, regardless of whether the total adds up to more than one.

To specify the anion of the mineral formula (in this case oxygen), select the element (or elements) in the periodic table list, and then click on the "Anions" button. This will add the element to the "Anions" list (label #7). Now enter the number of anions to the "Normalize to:" box (label #8) (in this case there are 8 oxygen atoms in the plagioclase formula). In the DHZ Worksheet, the cation atoms will be normalized to the 8 oxygen atoms.

Elements can be moved around within a site using the "Right >" and "< Left" buttons (labels #9 and 10). The purpose of moving the elements in the list is to obtain the desired order in the DHZ Worksheet. To arrange the order, select the element first and then click on the Right or Left button. To delete an element, select it and then click on the "Delete" button (label #11). The "Clear All" will delete the entire setup in the "by Site" Tab (label #12).

If the "Use for Search" checkbox is selected in the upper-right corner of the display, the setup in the "by Site" Tab will be used for the mineral match search. If this checkbox is unselected, all of the parameters set within this Tab will be ignored during the search. This allows the user to switch back

and forth using the site information as part of a search (or not) with the simple checking of a box and not having to reenter or delete all of the data.

Likewise, the individual site information will only be used if the checkbox next to that site (label #3) is checked. This allows the user to set up all of the sites for a particular mineral species, and by simply checking and unchecking boxes, either use them or not for particular searches.

The parameters setup in the "by Site" display can be stored using the "Save" button (label #14). The setup can be subsequently reused once they have been loaded, using the "Open" button (label #13). The name of the mineral setup (label #15) is obtained from the name of the file that was opened by the user.

"by Range" Tab

A general search of the mineral database can be run without any specific analysis for comparison. One method is to search the database using the compositional range for any number of elements (Fig. 21) in the "by Range" Tab.

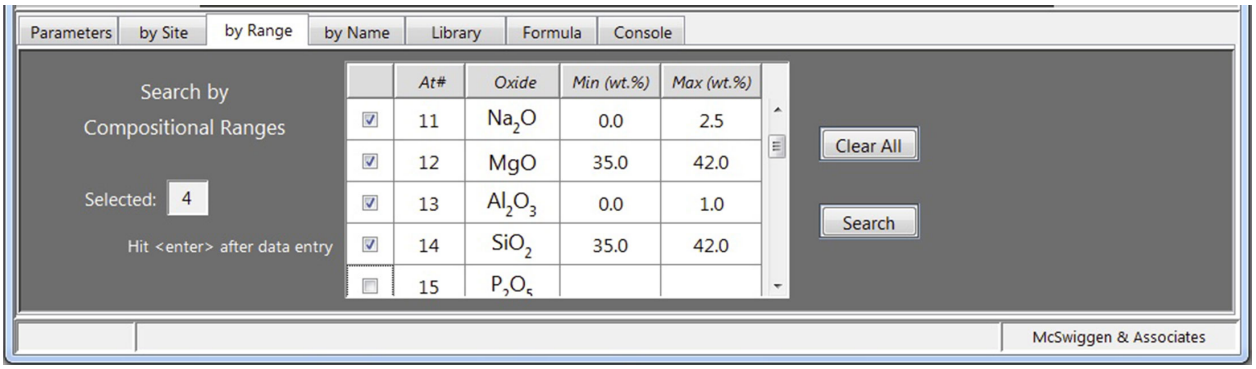


Figure 21. Layout of the "by Range" Tab. This Tab allows the user to search the mineral database by ranges in the element abundance.

The central table in the Tab is the element list from the periodic table. By default the elements are ordered alphabetically by the element symbol. This can be changed by clicking on the "At#" header, in which case the table will be ordered by the element's atomic number. The user can switch back and forth simply by clicking on the other column header.

When a checkbox for an element has been selected, the cursor will automatically position itself in the "Minimum" box for that element. The user can type in the minimum value for the element range, then click on the keyboard <tab> to move the cursor to the "Maximum" box.

When a value has been entered into one of the boxes in the table, the MINERALMATCH program will not recognize the value until the cursor has been moved from the box by either entering <tab> or <enter>, or by clicking on another box in the table.

Once all of the desired element ranges have been entered into the "by Range" list, hitting the "Search" button will run the search. Those minerals that match the specified ranges will be displayed in the Main Display (Fig. 6).

A total of 100 matched compositions can be displayed. If more minerals meet the entered criteria an error message will be displayed, and only the first 100 matches will be shown. The user can then further constrain the criteria to narrow the search.

The "Clear All" button is used to clear out all of the previously entered ranges from the periodic table list.

"by Name" Tab

A second way to search the mineral database without having a specific mineral analysis to compare with is to search by a mineral name, or by a mineral group name. Figure 22 shows some of the results from a search for all the minerals starting with "clino".

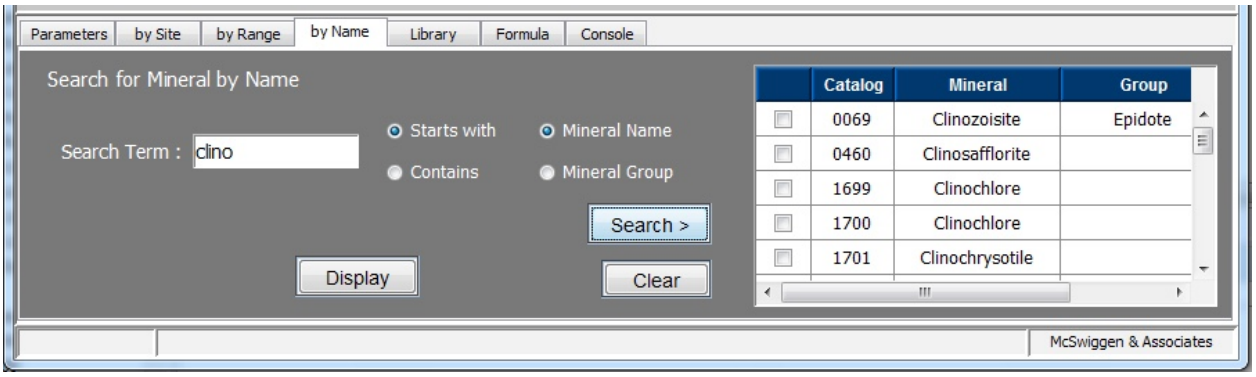


Figure 22. Layout of the "by Name" Tab showing the search for all minerals starting with the term "clino".

The term "clino" was entered into the Search Term box. The "Starts with" and "Mineral Name" options were selected. As a result, all of the mineral names beginning with "clino" were searched for when the "Search >" button was selected. All of the minerals that fit the criteria are displayed in the table to the right.

Up to 100 of these mineral compositions can now be displayed on the Main Display by checking the box next to the desired minerals and then clicking on the "Display" button.

Alternatively, all mineral names that contain the desired search term *anywhere* within the name can be found by using the "Contains" option. Likewise, the mineral group names can be searched using the "Mineral Group" option.

Creating User Libraries

The MINERALMATCH program contains a Master Library of thousands of mineral analyses (the exact number can be found in the "About" window; menu item >Options >> About). This Master Library is normally used when a search is run to find the closest match to a Target analysis. However, there are situations in which a smaller user-defined library might be the better database to search. For example, if a user wants to catalog the mineralogy of 1,000 Target analyses automatically and get consistent results for accurate statistics, a smaller user-defined library containing only a limited set of minerals might be more effective.

The user can define any number of User Libraries, but only one User Library can be open at any given time. By default, the Master Library is used for all mineral match searches (Fig. 23). To use a User Library, a new library must be created or an existing library must be opened.

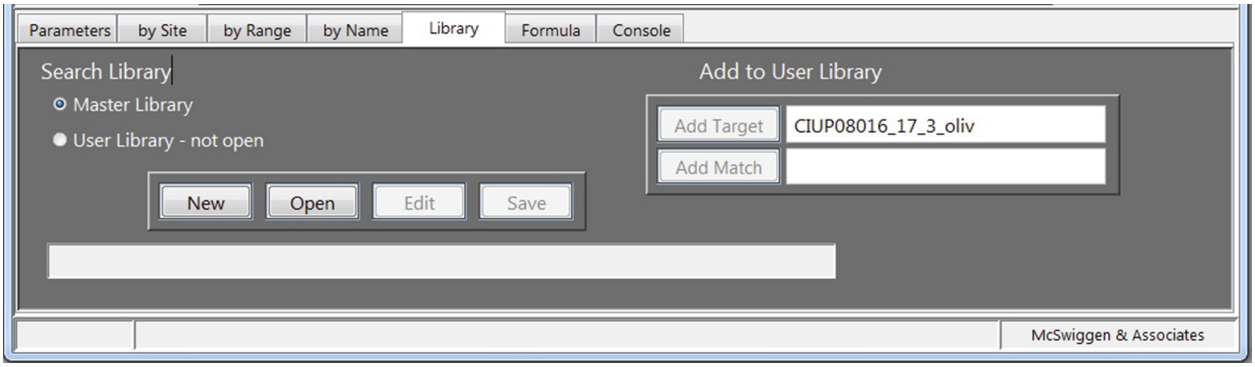


Figure 23. Layout of the Library Tab. By default the Master Library is selected for mineral match searches, but User created libraries can also be used.

To create a new User Library, click on the "New" button (Fig. 23). This will open the normal file chooser window (Fig. 24). Enter a new file name for this User Library.

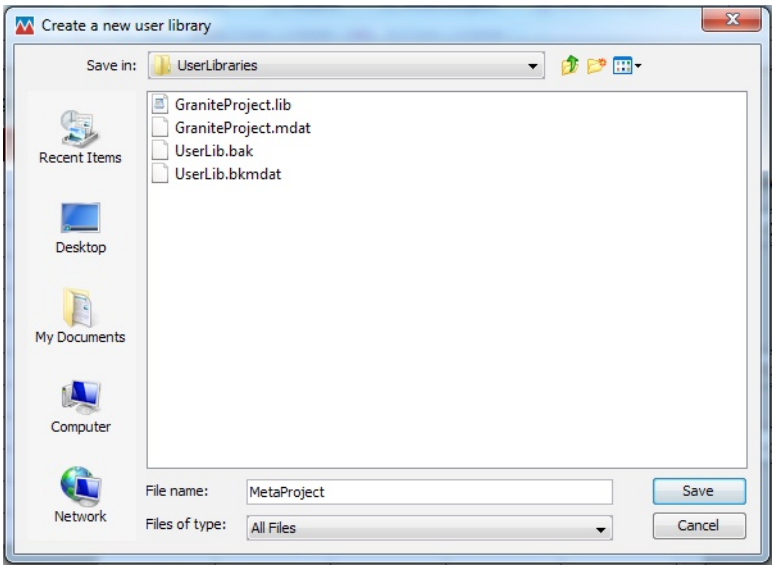


Figure 24. File chooser window to create a new User Library. In this example, the new library name will be "MetaProject".

Once a name has been added to the new file chooser and the window closed, the new User Library name and file path are displayed in the Library Tab (Fig. 25, label #1). However, at this point, the new User Library is still labeled as being "not open". This is because the User Library contains no data. Data can be entered into the User Library by either clicking on the "Add Target" or "Add Match" buttons.

When a new Target analysis has been displayed, the label for that analysis automatically gets added to the Add Target label in the Library Tab (Fig. 25). By clicking on the Add Target button, that composition along with its label gets added to the User Library. However, the Target label can be edited any time before the analysis gets added to the User Library.

Any of the matched mineral analyses can also be added to the User Library. When a matched mineral is selected in the Main Display, that mineral's name gets added to the Add Match label (Fig. 25). Clicking on the Add Match button then adds the composition and mineral name to the User Library. As with the Target label, the Match mineral name can also be edited before adding to the User Library.

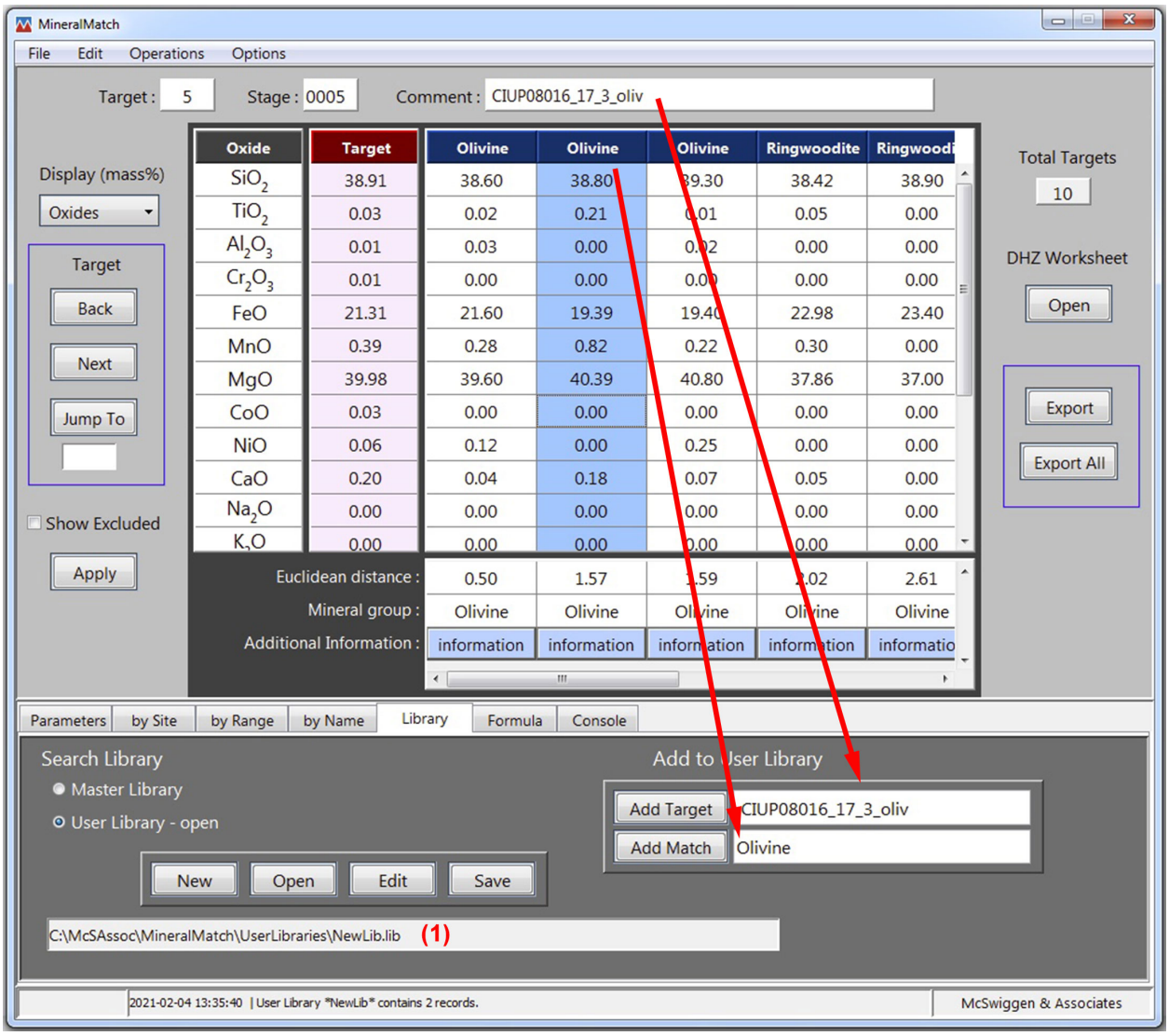


Figure 25. Layout of the Library Tab, along with the Main Display.

Once the User Library contains data, it can be selected as the active library. All searches after that will use that User Library instead of the Master Library.

After new mineral data has been stored to the User Library, it is important for the user to save that data to the library file. Simply click on the "Save" button **before** closing the program.

The contents of a User Library can be edited. Minerals can be deleted from the file, and the mineral names can be modified. However, the composition cannot be modified. To change the composition of a mineral, the old entry must be deleted and a new composition added.

To edit a mineral already in the User Library, click on the "Edit" button in the Library Tab (Fig. 25). This will open a window showing a list of all the minerals already in the User Library (Fig. 26).

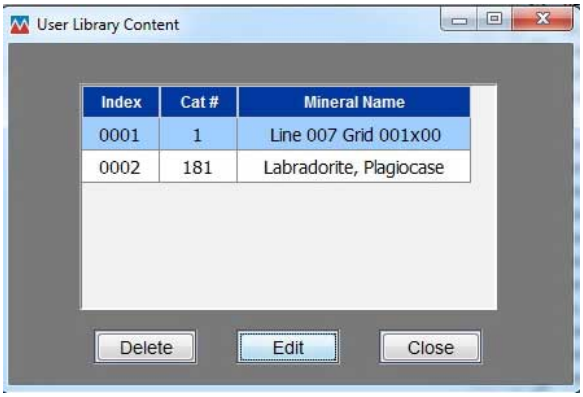


Figure 26. List showing the contents of the User Library.

To delete one of the mineral compositions, select the mineral in the list and click on the "Delete" button. To edit an existing mineral in the library, select the mineral and click on the "Edit" button. This will open the window shown in Figure 27.

In this window, the user can edit the mineral name or any of the other displayed information. However, remember to save the User Library to permanently store these changes.

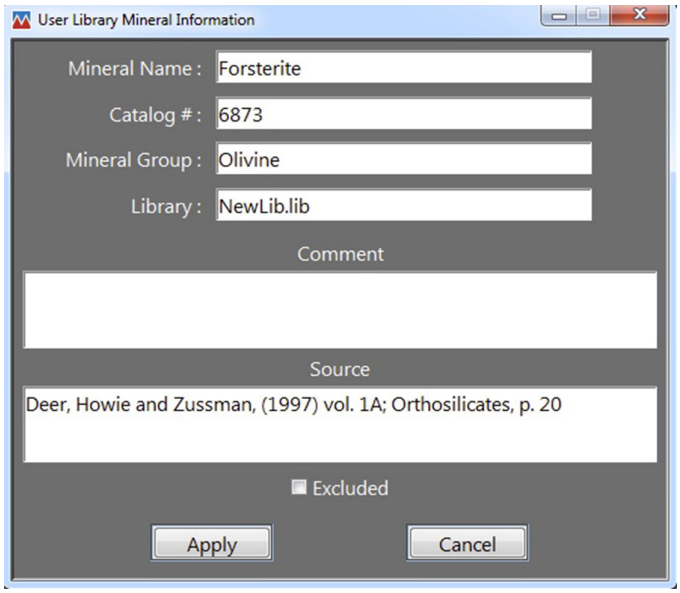


Figure 27. Mineral information window showing all of the metadata for a mineral in the User Library. The user can edit any of the metadata.

Now that the User Library has been created, or opened and populated with mineral data, it can be used for the mineral searches. Click on the "User Library" button in the Library Tab display (Fig. 25) to use this library in place of the Master Library.

Search for Mineral Formulas

Once an analysis has been matched with a specific mineral, it may be useful to have the formula for that mineral. The mineral formula provides useful information about how the sites within the mineral are filled, which in turns helps the user determine if the compositional match is really the correct mineral identification. The Formula Tab allows the user to search through a database of almost 5,000 mineral formulas (Fig. 28).

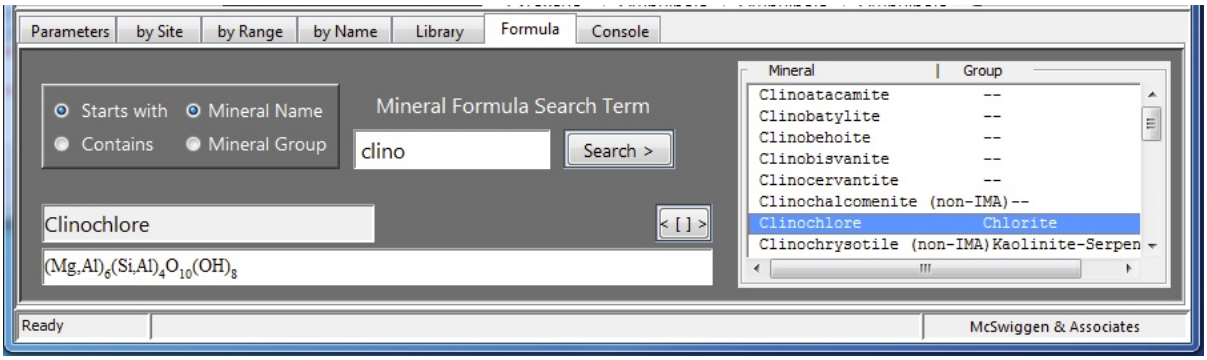


Figure 28. Layout of the Formula Tab.

To search for the mineral formula of a particular mineral, enter the search term into the appropriate box in the Formula Tab display. The search term can be the full mineral name or part of either the mineral name or the mineral group name. If the search term is the first part of the mineral name, click on "Starts with", or use the "Contains" option. Once the "Search >" button is clicked on, MINERALMATCH will list all of the minerals that fit those criteria. Scroll through the mineral list and then select the one mineral for which you want the formula displayed.

In the example above, the search term "clino" was used, and the mineral clinochlore was selected to display its formula.

To display the mineral formula in a larger font, click on the <[]> button. This will open the Mineral Formula window shown in Figure 29.

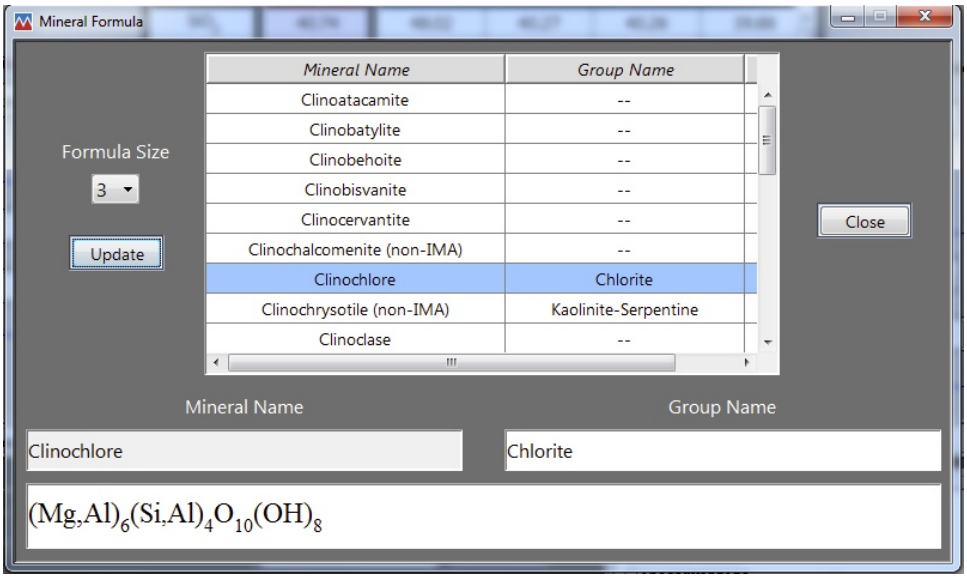


Figure 29. Mineral Formula window. This window allows for the display size of the formula to be enlarged.

The mineral formulas can be displayed in three different sizes. If the formula size has been changed, but the formula display has not changed, click on the "Update" button.

DHZ Worksheet

Once a mineral has been identified as a good match for an analysis, it may be helpful to see if the atom ratios fit that specific mineral formula. This is especially true if one is trying to choose between a few match options. The best match might not be the one with the smallest Euclidean distance, but the one with the closest agreement to the atomic ratios defined by the formula.

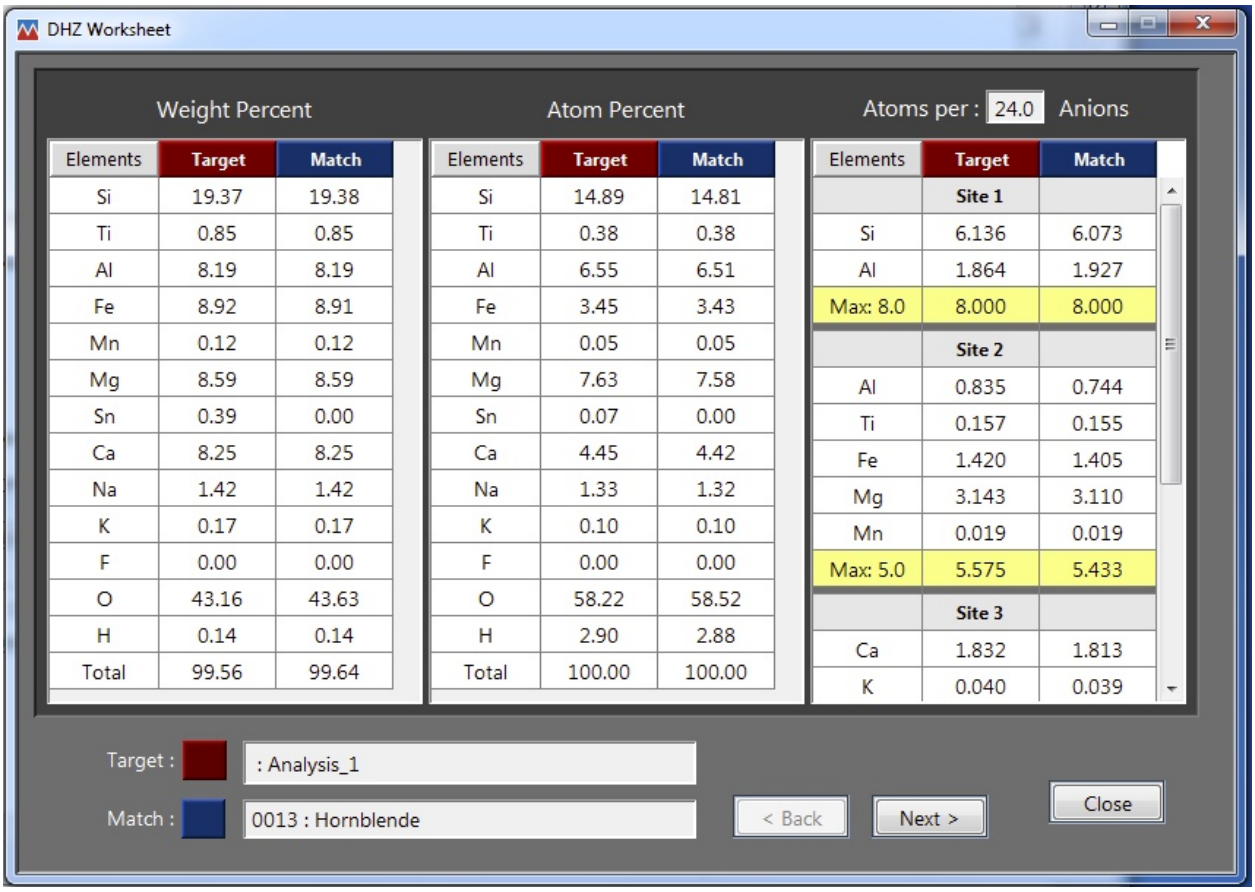
The DHZ worksheet (short for Deer, Howie and Zussman) shows the comparison between the Target and Match analyses for the mass percent, atom percent, and the number of atoms per unit formula. The atoms per unit formula is then grouped by the sites defined in the "by Site" Tab. This is the best way to determine if the two analyses fit the same mineral formula.

Before displaying the DHZ Worksheet, check the "by Site" Tab to make sure it is configured for the mineral species in question. If there is any doubt, look up the mineral formula in the Formula Tab. If still in doubt, consult the excellent multi-volume references entitled "Rock Forming Minerals" by the authors: Deer, Howie and Zussman (see References). These references are generally considered to be the final word on rock forming minerals.

In the DHZ Worksheet, the first columns of data show the analyses in mass percent. The user can display either the oxide mass percent or the elemental mass percent. This choice is selected in the Main Display in the Display (mass%) drop down menu (Fig. 8, label #1). Before opening the DHZ Worksheet, first decide which Match mineral the Target should be compared to. If no Match mineral is selected, then the first one listed will be displayed in the worksheet. Otherwise, whichever Match column is selected is displayed.

To open the DHZ Worksheet, click on the DHZ Worksheet Open button in the upper-right corner of the Main Display. This will open the window shown in Figure 30. The worksheet is divided into three columns. Each compares the Target analysis with the Match analysis. On the left is the weight percent by

either oxide or by element. In the center is the comparison of the atom percent, and on the right is the table of atoms per unit formula grouped by mineral site.



Elements	Target	Match
Si	19.37	19.38
Ti	0.85	0.85
Al	8.19	8.19
Fe	8.92	8.91
Mn	0.12	0.12
Mg	8.59	8.59
Sn	0.39	0.00
Ca	8.25	8.25
Na	1.42	1.42
K	0.17	0.17
F	0.00	0.00
O	43.16	43.63
H	0.14	0.14
Total	99.56	99.64

Elements	Target	Match
Si	14.89	14.81
Ti	0.38	0.38
Al	6.55	6.51
Fe	3.45	3.43
Mn	0.05	0.05
Mg	7.63	7.58
Sn	0.07	0.00
Ca	4.45	4.42
Na	1.33	1.32
K	0.10	0.10
F	0.00	0.00
O	58.22	58.52
H	2.90	2.88
Total	100.00	100.00

Elements	Target	Match
	Site 1	
Si	6.136	6.073
Al	1.864	1.927
Max: 8.0	8.000	8.000
	Site 2	
Al	0.835	0.744
Ti	0.157	0.155
Fe	1.420	1.405
Mg	3.143	3.110
Mn	0.019	0.019
Max: 5.0	5.575	5.433
	Site 3	
Ca	1.832	1.813
K	0.040	0.039

Figure 30. DHZ Worksheet showing the comparison of the Target and Match analyses in terms of the oxide (or element) mass percent, atom percent, and atoms per unit formula grouped by the sites configurations.

The user can step through the entire set of Match minerals by using the "Next" and "Back" buttons in the window.

To compare another Target analysis, close the DHZ Worksheet and then select a new Target before reopening the worksheet.

Exporting Results

The final Match result can be exported jointly with the Target analysis. This can be done one at a time, allowing the user to select the best Match mineral first, or it can be done automatically for the entire set of Target analyses. If it is done automatically in a batch process the software will automatically pick the Match with the smallest compositional difference.

Single Point

Every time a new set of Target data is loaded into the software, information on the list of elements in those analyses is output to the Console Tab window. The form in which this element header information is written depends on the form the analysis was originally read into the program. Therefore, if the analysis was in an oxide form in the original file, the element header output to the console will be in the oxide form.

After that, every time the user clicks on the "Export" button in the Main Display, the composition of the Target analysis will be output to the Console along with the mineral name of the selected Match mineral. If the user does not select a Match mineral, the output mineral name will be the first one in the list with the smallest compositional difference.

The Target analysis will always be output in the same element or oxide form as they were originally read into the program. The Display (mass%) dropdown menu selection will not change this.

After the mineral name, the Euclidean distance for the Match will also be displayed. This allows for a permanent record of the nearness of the match.

Batch Processing

Batch processing of the analytical data can be used when a large number of analyses need to be processed. This will in turn give the best results if preliminary work has been already done to identify all of the possible minerals that might be encountered in the project. This subset of Match minerals should be loaded into a User Library and that library should be selected as the active library.

After all the Target analyses have been loaded into the program, simply click on the "Export All" button in the Main Display window. Each target analysis will be output to the Console window along with the closest fit mineral match from the User Library. This will allow the user to quickly classify the mineralogy of the set of Target analyses.

The results from the Console window can now be saved to an Excel spreadsheet.

Console Window

The Console window is a simple text window. The content of which can be copied, pasted, edited or cleared, using the Edit menu. The contents of the Console window can also be saved to an Excel spreadsheet. Go to the File >> Save As menu item and the standard Save window will open (Fig. 31). The user can save the data in one of three formats:

- xls : Old Excel format.
- xlsx : New Excel format.
- txt : Tab separated text file.

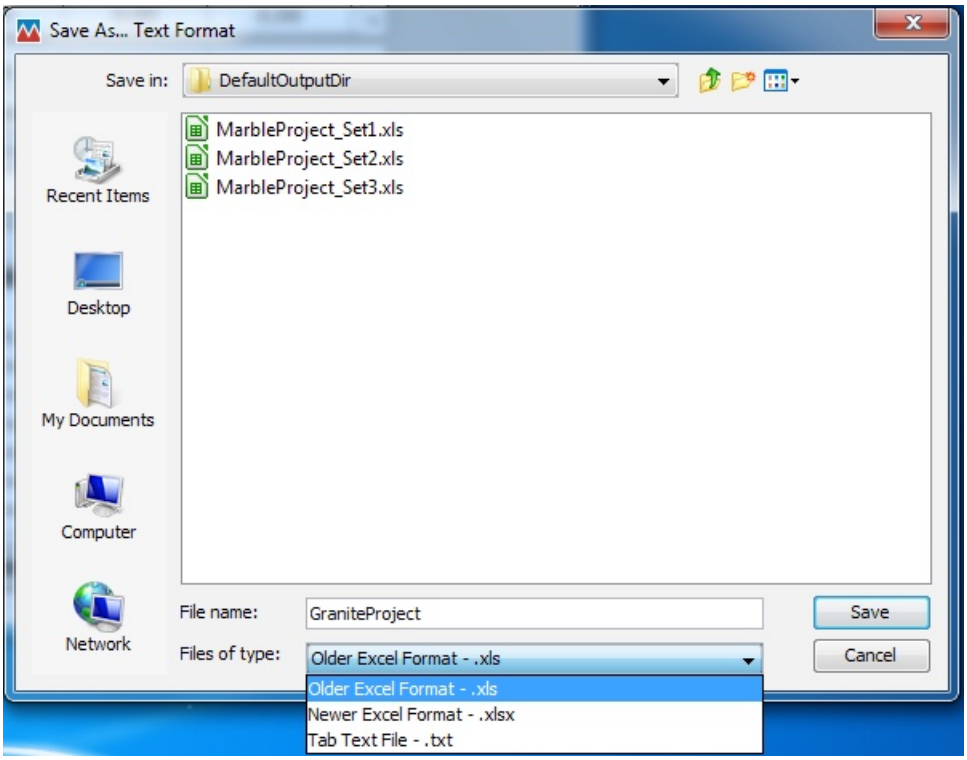


Figure 31. Save window for the Console data.

Options

In the Options menu there are three sets of controls that a user should be familiar with.

Options Window

The Options window contains three parameters that the user can modify (Fig. 33). First is the Output Element Order. This controls the order in which the elements are displayed in the Main Display and in the DHZ Worksheet. There are four options. Using the "Silicates" option, the elements are ordered in the output that follows the general sequence used by Deer, et al. (1992). Si or SiO_2 is first, followed by those elements that can substitute for Si. Last in the list will be extra oxygen, water, and any other anions.

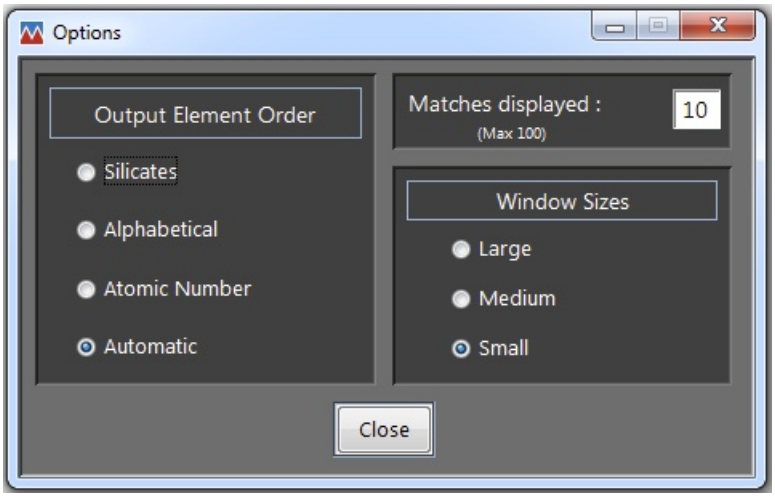


Figure 33. Options window.

If the elements are ordered alphabetically, they are ordered based on their symbol letters not the spelling of their names. Alternatively, elements can be ordered based on their atomic number. The last and ***default*** option is "Automatic". If this is selected and there is greater than 5 wt.% Si, the

software will display the elements in the "Silicates" order. Otherwise the elements will be ordered alphabetically by symbol.

A second variable in the Options window (Fig. 33) that the user can set is the maximum number of Matches to be displayed in the Main Display at any one time. The default cutoff is 10. This can be increased up to 100.

Lastly, the user can set the size of the program window itself. Monitors come in different sizes and with different resolutions. A program window might look perfect on one and might be completely unreadable on another. Therefore the user can select between three different window sizes. With each window, the font size and components of the window will change. Start with the smallest window size and work up to the one that is most readable for the monitor that it is being used. Once the display size has been changed, the program ***must*** be restarted for it to take effect.

Changing Oxide Types

The MINERALMATCH program can only work with one set of oxides at a time. Therefore, for example, the user can choose either FeO or Fe_2O_3, but cannot use both at the same time. To view the list of oxide forms being used, select the *>Options >> Oxide Type* menu item. The Oxide States window will open (Fig. 34).

The user can change their preferred oxide form for many elements. Simply click on the "Periodic Table" button and a window will be displayed showing a periodic table with the default oxide forms (Fig. 35). To change the preferred oxide state, click on the element of interest. If there are other oxide options, then a dropdown menu will display the alternative options. Select the preferred oxide state.

If a new set of Target analyses is loaded into the program as oxides, the software will use that list of oxides as the preferred oxide state.

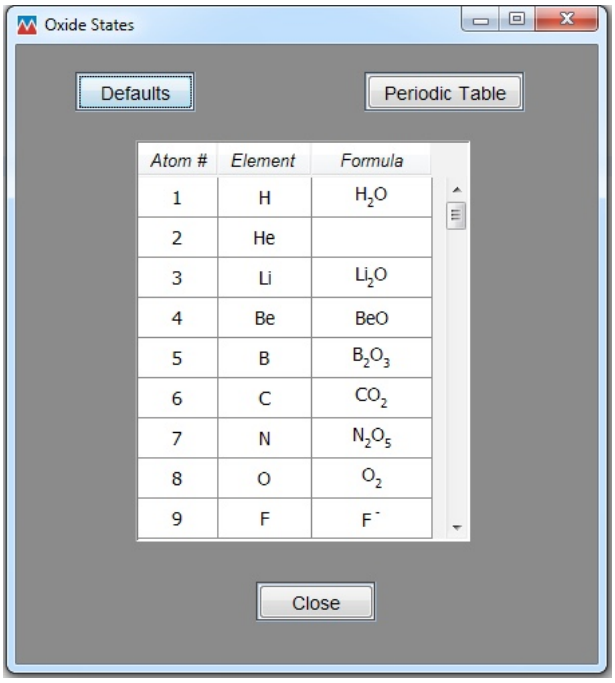


Figure 34. List of oxide states being used by the software.

Therefore to change the display oxides, it must be done **after** the Target analyses have been input. Otherwise it might get reversed to a different set of oxides once the analyses have been imported.

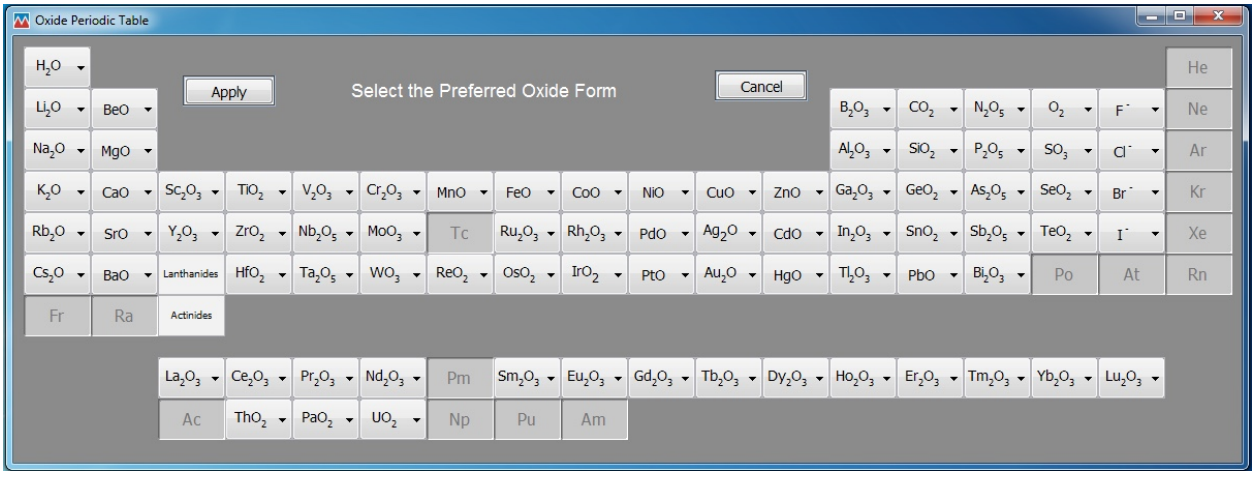


Figure 35. Periodic table of the display oxides. Users can change their preferred oxide form for an element in this window.

The oxide forms that are being used by the software can be reset back to the original default values by clicking on the "Defaults" button in the Oxide States window (Fig. 34).

Troubleshooting

Installing the Software

A Java JRE (Java Runtime Environment) must be installed on the computer in order to run the MINERALMATCH or the installer program. To determine if the JRE is installed, do the following:

1. Go to the Start Menu and type "cmd" in the search box (Fig. 36). This will bring up the Command Prompt program. Click on it to run.

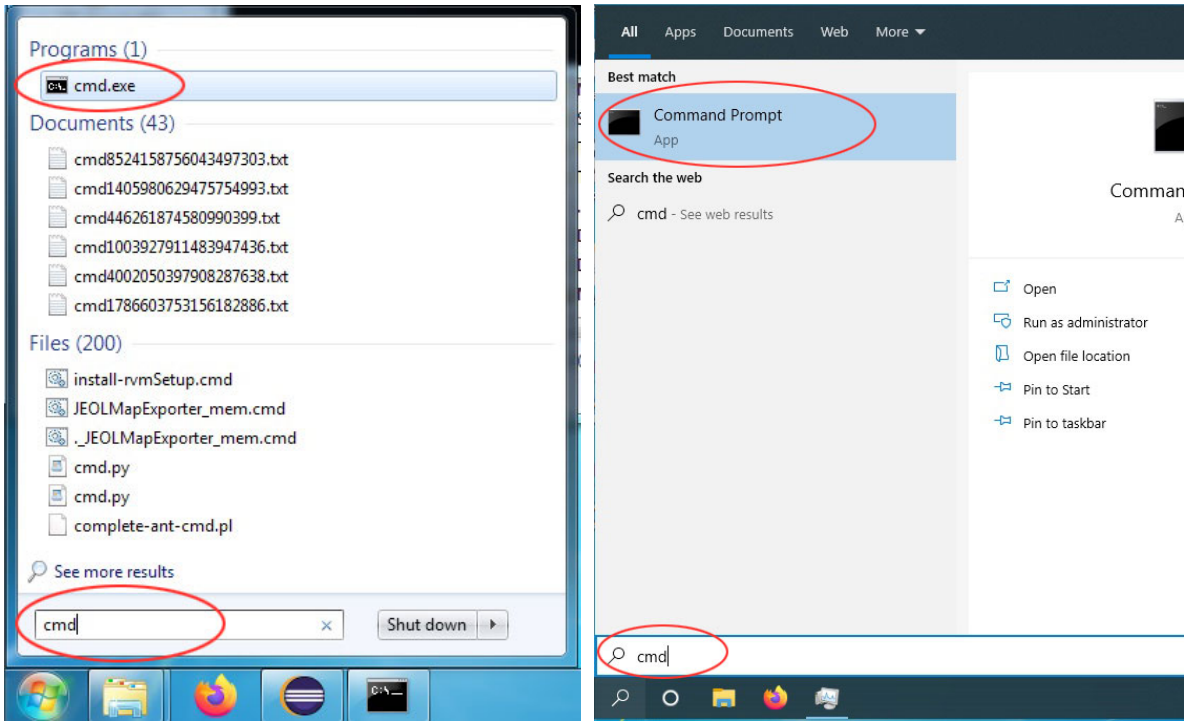


Figure 36. Search for and run the cmd.exe program using the Search box in the Start window; (a) Windows 7, and (b) Windows 10.

2. Type into the Command window at the prompt, "java -version" (Fig. 37). If it doesn't come back with the version information, then Java is not installed and must be installed by the user before the MINERALMATCH installer can be run.

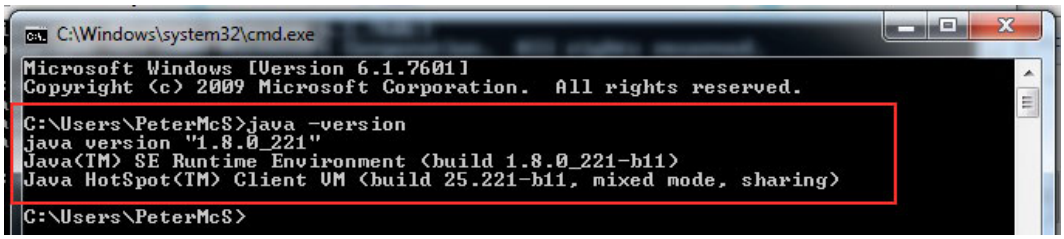


Figure 37. Version information for the Java Runtime Environment (JRE) installed on the computer.

If it is not installed, install it before trying to run the MINERALMATCH installer. Copies of the Java JRE can be found in the Java directory on the CD ready for installation - one each for the 32-bit and 64-bit systems.

Whether your system is a 32-bit or 64-bit operating system can be determined from the Control Panel.

Start Menu >> Control Panel >> System >> About (Windows 10)
Start Menu >> Control Panel >> System (Windows 7)

To install the MINERALMATCH software, insert the accompanying CD into the appropriate drive, and plug the accompanying dongle into an existing USB port.

Now execute the following steps:

1. Run the program: MineralMatch_Installer.exe
2. Choose between (a) a full installation, or (b) a re-install. The full installation includes the complete content of the MineralMatch directory. The re-install option will only copy the files required to run the program. Thereby, user data outside the "ProgramData" directory will not be overwritten. The initial installation requires the full installation.
3. Click on the Start button and, when prompted, choose whether to include a desktop shortcut or a Start menu shortcut.
4. MineralMatch can now be run by either clicking on one of its shortcuts, or by using the path below.

   C:\McSAssoc\MineralMatch\MineralMatch.exe

Program Won't Start

(1) Missing Dongle

The program MINERALMATCH will not run unless the accompanying dongle is plugged into one of the USB ports on the computer. If the dongle is plugged into the computer, try unplugging it and reconnecting it to the USB port. If this does not resolve the problem, contact support below (p. 55).

(2) Program is already open

Only one instance of MINERALMATCH can be run at a time. If the program is already open, an error message will be displayed warning of that fact. If the error message "MINERALMATCH is already open" occurs when there is no other such instance open, then it is possible that one of the configuration files has been corrupted. To correct for any corrupt configuration files, run the Reset-MINERALMATCH program. If shortcuts to the program are not on the desktop or in the Start menu, the program can be found at:

C:\McSAssoc\MineralMatch\ProgramData\Reset-MINERALMATCH

Run the program and click on "Execute" (Fig. 38).

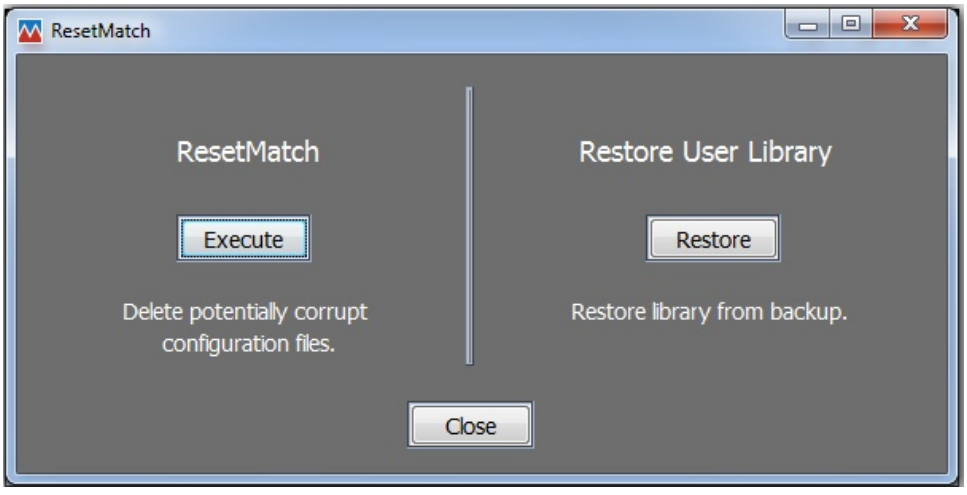


Figure 38. Control page for the Reset-MINERALMATCH *program.*

Corrupt User Library

When a User Library is open, a backup is automatically created. If the original User Library should get corrupted and cannot be opened, the backup can be converted into the User Library. To do this, run the Reset-MINERALMATCH program (Fig. 38), and click on the "Restore" button.

Select the backup to the desired User Library (suffix on the file will be ".bak") (Fig. 39).

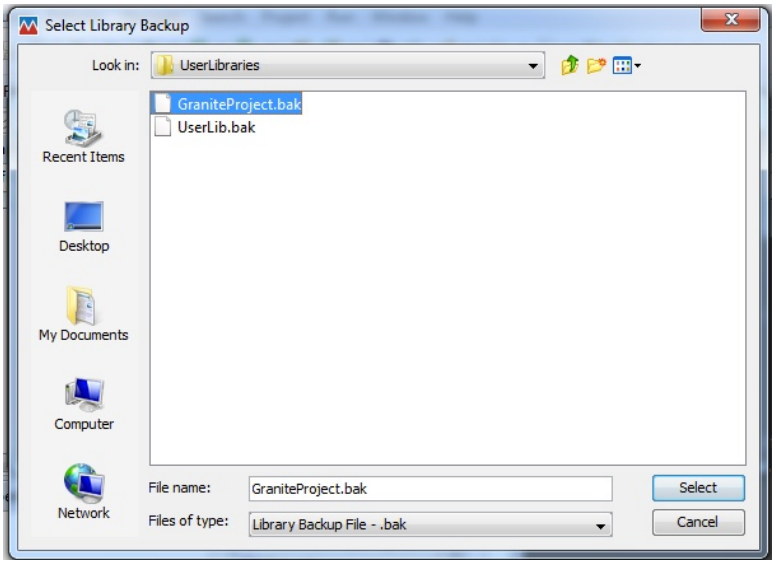


Figure 39. Select the User Library backup to be restored.

Only one backup is ever made of an individual User Library. Therefore if a library needs to be restored, it must be done before that particular library gets opened again in the MINERALMATCH program.

Managing Shortcuts

Shortcuts to the MINERALMATCH and Reset-MINERALMATCH programs can be installed onto the desktop and into the Start menus automatically during installation. If this option is selected, these shortcuts will be installed in the following users paths.

desktop :
C:\Users\<username>\Desktop
Start menu :
C:\Users\<username>\AppData\Roaming\Microsoft\Windows\Start Menu

The shortcuts on the desktop and in the Start menu can be made available to all users by moving them to the following directories.

desktop :
C:\Users\Public\Public Desktop
Start menu :
C:\ProgramData\Microsoft\Windows\Start Menu\Programs

If the shortcuts were not installed during the installation, they can later be moved from this directory:
C:\McSAssoc\MineralMatch\ProgramData\ShortCuts
to the appropriate directories listed above.

Windows 10 Crashes

Windows 10 can cause some peculiar behavior. When its display is set to enlarge to 125% of normal, it can cause crashes to unrelated programs. In the MINERALMATCH program, if crashes occur when the "by Site", "by Range" or "by Name" tab are selected, the first suspect should be the display settings of Windows 10. Check the display settings to make sure enlargement is not set to 125% (Control Panel >> System >> Display >> Scale and layout), where it says "Change the size of the text, apps, and other items". No problems have been found when enlargement is set to 100% or 200%, but problems might occur at 125%.

Similar problems have not been found in Windows 7.

Registration and Support

Register your copy of the MINERALMATCH software to ensure you get the latest upgrades to the application and updates to the mineral database. Send your name, institution name, and email address to:

Peter McSwiggen (PMcS@McSwiggen.com)

Support for the MINERALMATCH program is also provided at the same address. Feel free to send any description of problems, bugs, suggestions, or questions.

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