



# CSpace: an integrated workplace for the graphical and algebraic analysis of phase assemblages on 32-bit wintel platforms<sup>☆</sup>

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## Abstract

CSpace is a program for the graphical and algebraic analysis of composition relations within chemical systems. The program is particularly suited to the needs of petrologists, but could also prove useful for mineralogists, geochemists and other environmental scientists. A few examples of what can be accomplished with CSpace are the mapping of compositions into some desired set of system/phase components, the estimation of reaction/mixing coefficients and assessment of phase-rule compatibility relations within or between complex mineral assemblages. The program also allows dynamic inspection of compositional relations by means of barycentric plots. CSpace provides an integrated workplace for data management, manipulation and plotting. Data management is done through a built-in spreadsheet-like editor, which also acts as a data repository for the graphical and algebraic procedures. Algebraic capabilities are provided by a mapping engine and a matrix analysis tool, both of which are based on singular-value decomposition. The mapping engine uses a general approach to linear mapping, capable of handling determined, underdetermined and overdetermined problems. The matrix analysis tool is implemented as a task “wizard” that guides the user through a number of steps to perform matrix approximation (finding nearest rank-deficient models of an input composition matrix), and inspection of null-reaction space relationships (i.e. of implicit linear relations among the elements of the composition matrix). Graphical capabilities are provided by a graph engine that directly links with the contents of the data editor. The graph engine can generate sophisticated 2-D ternary (triangular) and 3D quaternary (tetrahedral) barycentric plots and includes features such as interactive re-sizing and rotation, on-the-fly coordinate scaling and support for automated drawing of tie lines. © 2000 Published by Elsevier Science Ltd.

*Keywords:* Composition space; Coordinate mapping; Matrix analysis; Barycentric plots; Singular value decomposition

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<sup>☆</sup> Code available at <http://www.iamg.org/CGEditor/index.htm> and at <http://www.ugr.es/~cspace>

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## 1. Introduction

Manipulating the compositional variables that define the “composition space” of chemical systems (either homogenous or heterogeneous) is frequently required to solve or clarify many mineralogical and petrologic

problems (Spear et al., 1982). Applications differ widely, from illustration to sophisticated analysis and modeling of extensive phase relationships, all of which are currently facilitated by the general availability of reliable techniques of mineral and rock analysis. However, manipulating compositional variables and inspecting compositional relationships can be time-consuming, particularly when the need arises in working with large natural data sets and in the application of the more advanced graphical and algebraic techniques. Fortunately, many of these tasks are amenable to computer treatment and, following theoretical work by Thompson (1957), Korzhinskii (1959), Greenwood (1967) and others, a number of algorithms and specialized computer programs have been devised to help with many specific applications and issues (e.g., Albarède and Provost, 1977; Ball and Robin, 1990; Fisher, 1989, 1993; Fletcher and Greenwood, 1979; Greenwood, 1968, 1975; Pigage, 1976; Powell, 1990; Rock and Carroll, 1989; Rock et al., 1991; Spear, 1980; Spear et al., 1991).

CSPACE is a 32-bit Windows<sup>2</sup> application aimed at further facilitating the use of state-of-the-art techniques in the analysis of compositional relationships by providing a self-contained and interactive data management and analysis environment. The program integrates a set of general tools for the algebraic manipulation and modeling of  $n$ -dimensional composition space and includes advanced capabilities for the graphical representation of composition relations using barycentric plots. CSPACE is primarily intended as a research aid in the analysis of phase assemblages; its functionality, however, extends to many related mineralogical and geochemical purposes and should prove equally suitable for training. The purpose of this paper is to introduce the main program features, with emphasis on the underlying procedures and algorithms. Program usage is described in more detail in the online documentation (help) that is linked to the program itself.

## 2. Main interface elements

CSPACE's main interface elements consist of three resizable linked windows, titled *CSPACEData*, *CSPACEGraphs* and *TextPad*, each having specific command menus and purposes that are briefly introduced in the following sections. Other important interface elements include a number of dialogs that are presented to the

user in response to menu commands that require additional input. These dialogs and their usage are described in the online documentation.

### 2.1. CSPACEData window

The *CSPACEData* window (Fig. 1) is the main program window and provides access to application-level features such as global options, help browsing and program exit. As its name implies however, the main purpose of the *CSPACEData* window is data management and manipulation. These tasks are handled by the *DataSheet*, a spreadsheet-like grid that stores a two-dimensional data table (i.e., data that is organized into cases and variables, arranged into rows and columns). The *DataSheet* is both an editor and the live repository of data that is to be processed by CSPACE. As an editor, it allows creating, opening, editing and saving data files, and its usage is similar to that of standard spreadsheets, including in-place editing of cell values, range selection procedures and clipboard exchange of data to/from most commercial spreadsheets or text editors. The *DataSheet* cells, however, only contain values (either numeric or text), and columns are referred to by the names of the contained variables. As a data repository, the *DataSheet* includes facilities for marking or selecting the cases and variables that are to be used at any time for plotting or manipulation. Operation on the data is interactive. Once the data to be acted upon are defined, the user can select a command or procedure from menus, then examine (and eventually save) the results.

### 2.2. CSPACEGraphs window

The *CSPACEGraphs* window (Fig. 2) houses the graph engine of CSPACE. The essential controls on this window are its toolbar and the plot area. The toolbar facilitates selecting plot variables and some popular graph options (such as whether to display point labels or tie lines). On-screen display in the plot area faithfully represents what is printed, either actual size or scaled to fit the window. Clicking the tabbed control at the bottom of the plot area allows instantly changing the type of plot displayed.

Working with plots is just a matter of selecting which variables (i.e. *DataSheet* columns) should be plotted and adjusting plot appearance. The graphs can be configured for a variety of properties and settings by means of dialogs or commands that are accessible from the main menu of the *CSPACEGraphs* window. The File and Edit menus give access to commands for printing, exporting and clipboard-copying the displayed graph. Either exporting or copying can be done in vector (metafile) or raster (bitmap) formats. The

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<sup>2</sup> Windows is a trademark of Microsoft Corporation. To run CSPACE, a PC-compatible machine using either Windows 9x or Windows NT (4.0 or higher) is required. CSPACE is available from the Web at <http://www.ugr.es/~cspace>.

	Label#	SiO2	MgO	FeO	SiO2+	MgO+	SiO2#	MgO#	FeMg-1#
1	Qtz	0.99	0	0	1	0	0.999999	0	0
2	Opx	1.01	0.251	0.748	1	1	1.000001	0.99999995	0.74849998
3	Ol	1.005	0.498	1.502	1	2	1.0000005	2	1.502
4	SiO2'	1	0	0	1	0	1	0	0
5	MgO'	0	1	0	0	1	0	1	0
6	FeMg-1	0	-1	1	0	0	0	0	1

5 6 6

Fig. 1. *CspaceData* window, with view of DataSheet after performing constrained mapping of hypothetical quartz (Qtz), orthopyroxene (Opx) and olivine (Ol) analyses from SiO<sub>2</sub>-MgO-FeO to SiO<sub>2</sub>-MgO'-FeMg<sub>-1</sub> molar coordinate systems. Variables tagged with '+' were added to original data to constrain additive components in new set by means of differential weighting according to procedure suggested by Fisher (1993), from which example is taken. Note that transformation matrix is specified by last three cases (selected). Numeric values along message bar at bottom of window indicate (from right to left) number of cases (a) contained in DataSheet, (b) selected for plotting or mapping and (c) those that could actually be plotted using current set of plot variables (in example, all cases minus one defining composition of MgFe<sub>-1</sub> exchange component that has barycentric zero sum). Note that current plot set is marked with capital letters along header row containing variable names.

capabilities of the graph engine are described in a later section.

### 2.3. TextPad window

The *TextPad* window (Fig. 3) contains a simple, line-oriented, text editor, similar to the Windows Notepad. Unlike the Windows Notepad, however, the *TextPad* can handle large files and has no option for wrapping lines. The *TextPad* main function is as the location where results are output by the procedures under the Matrix menu of the *CspaceData* window, although it can be used as a standard editor for existing files, as a scratchpad for notes or temporary data, or even to create or edit *Cspace* data files as an alternative to the DataSheet itself.

### Algebraic manipulation and analysis of *n*-dimensional composition space

*Cspace*'s algebraic capabilities revolve around the notion of "composition space" (Spear et al. 1982; Thompson, 1982a), which refers to a Cartesian space whose coordinates represent the amounts of the chemical species or components. Within a given composition space, specific compositions are regarded as coordinate locations with as many dimensions (i.e. coordinates) as the number of components used to describe them. Components are defined in terms of their chemical for-

mula and unit of measurement and, as expected for an orthogonal Cartesian axis, they should be able to vary independently from each other (i.e., be linearly independent). For a heterogeneous system containing *n* phases, for example, composition space can be mathematically defined from the Phase Rule as the range of **A** (see below) in the context of a linear system of equations of the type

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}, \quad (1)$$

where **A** is a *m* by *n* matrix describing the composition of the *n* phases (arranged into columns) in terms of *m* system components (arranged into rows), and both **x** and **b** are vectors that equally describe the composition of the system in terms of the proportions of the *n* phases and *m* system components, respectively (Fisher, 1989). The notion of composition space is particularly useful because, as noted by Spear et al. (1982), almost all the petrologic applications of linear algebra depend on appropriate handling of "mapping" systems of equations such as Eq. (1), notwithstanding the different ways in which problems can be formulated. In general, one will be interested in solving the system of equations to express compositions in terms of an alternate component set, and or in assessing the properties of matrix **A**, such as its effective range and any implicit linear relations among the compositions described by its columns. For these purposes *Cspace* provides two generic tools: the Mapping Engine (ME) and the Matrix Analysis Wizard (MAW), each being specifi-

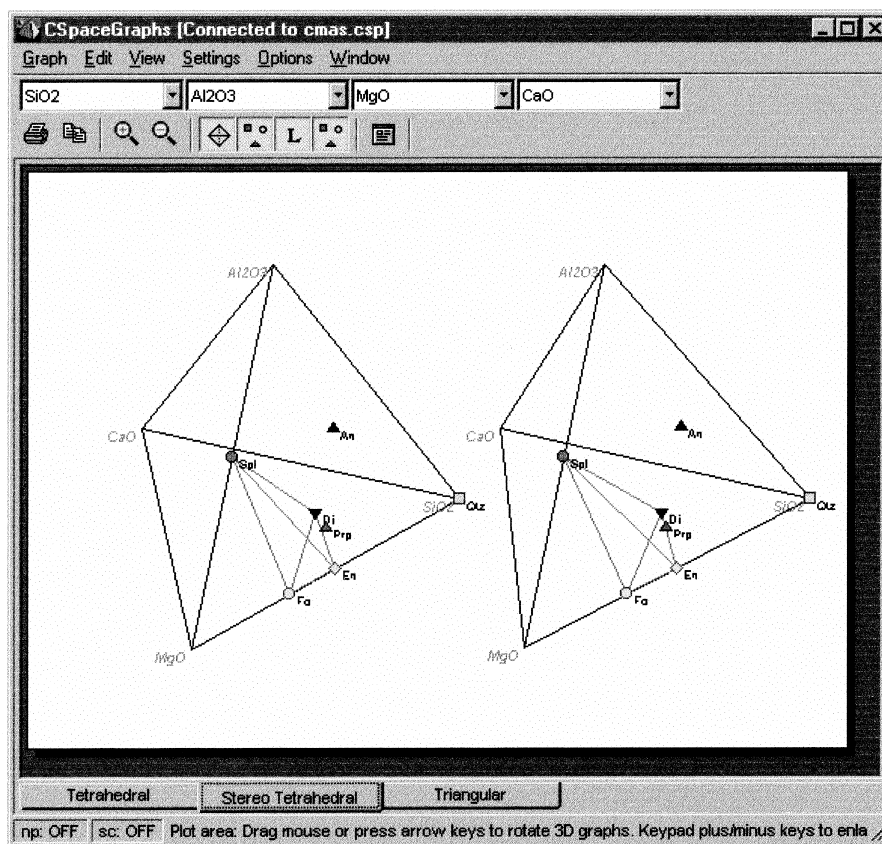


Fig. 2. *CspaceGraphs* window, showing plot area with example stereoscopic plot of phases within CMAS system. Note that current plot variables (from those contained in DataSheet) are specified in comboboxes located in toolbar. Clicking tabs along bottom of plot area changes type of plot displayed. Indicators at bottom-left of window show whether optional plotting of ‘negative’ points (np) and coordinate scaling (sc) is active.

cally adapted for multiple coordinate mapping and matrix modeling and analysis, respectively. Although primarily intended for the analysis of phase assemblages, the ME and the MAW impose no constraints to their use and should be flexible enough for a wide range of geochemical applications. Still, a basic understanding of their common fundamental algorithm (SVD) and general behavior is required. A brief introduction to these is made next.

### 3.1. Matrix subspaces and SVD

Textbooks on linear algebra often describe matrix  $\mathbf{A}$  of Eq. (1) as a kind of operator that “maps” (translates) one location between Cartesian spaces that differ with regard to the coordinate sets used (i.e., it defines an operation that is called a linear mapping from vector space  $\mathbf{x}$  to vector space  $\mathbf{b}$ ). In translating between these spaces, however, much depends on the relationship between both coordinate sets as portrayed by the properties of matrix  $\mathbf{A}$ . If  $\mathbf{A}$  is square and non-singular

then all of the  $\mathbf{b}$  space can be “reached” by  $\mathbf{A}$ , so that any location in space  $\mathbf{x}$  can be uniquely mapped into a corresponding location in  $\mathbf{b}$ . If  $\mathbf{A}$  is singular, however, then there is a portion of space  $\mathbf{b}$  that cannot be “reached” by  $\mathbf{A}$ , and “points” in space  $\mathbf{x}$  cannot be uniquely mapped into space  $\mathbf{b}$  but rather into an indefinite position with regard to the corresponding subspace of  $\mathbf{x}$  that cannot be mapped. This latter subspace is often referred to as the *null space* of  $\mathbf{A}$  and its number of dimensions is the *nullity* of  $\mathbf{A}$ . The subspace of  $\mathbf{b}$  that can be reached by  $\mathbf{A}$ , on the other hand, is termed the *range* of  $\mathbf{A}$  and its dimensions are the *rank* of  $\mathbf{A}$  or  $r(\mathbf{A})$ . Rank plus nullity always equal  $n$ , so non-singular matrices have  $\text{rank} = n$  and singular (or rank-deficient) matrices have  $\text{rank} < n$ . Note that rank and nullity refer to the number of linearly independent vectors (analogous to orthogonal Cartesian axes) that can be found in each subspace and would be sufficient to describe any location within it. The set of independent vectors spanning the range fully defines the space that can be reached by  $\mathbf{A}$  (i.e. the composition space),

whereas the analogous vector set spanning the null space specifies existing linear dependencies in  $\mathbf{A}$  (if any). As pointed out by Fisher (1989), the null space is analogous to the reaction space of Thompson (1982b) in that it could represent “reaction” relationships among the elements described by the columns of  $\mathbf{A}$  when they represent phase components. More generally, null-reaction space simply represents linear compositional relations, analogous to mass-balances, that are implicit in the matrix of compositions  $\mathbf{A}$ . Algebraic analysis of matrix  $\mathbf{A}$  (that is, assessing its range and finding and inspecting any implicit linear relations) is thus a powerful technique in deciphering compositional relations within systems of any complexity. For that purpose, CSpace uses singular value decomposition (SVD) which was first introduced to petrologic applications by Fisher (1989; see this paper for a discussion of the relative merits of SVD with regard to other algebraic techniques). SVD encompasses a most useful family of methods in linear algebra which derives from a theorem that states that any  $m$  by  $n$  matrix  $\mathbf{A}$  ( $m > n$ ) can be written as the product of an  $m$  by  $n$  column-orthogonal matrix  $\mathbf{U}$ , an  $n$  by  $n$  diagonal matrix  $\mathbf{W}$  with positive or zero elements, and the transpose of an  $n$  by  $n$  orthogonal matrix  $\mathbf{V}$ :

$$\mathbf{A} = \mathbf{U} \cdot \text{diag}(\mathbf{W}) \cdot \mathbf{V}^T. \quad (2)$$

The usefulness of SVD derives from several of its fundamental properties. The SVD of a matrix can always be obtained, whether it is singular or not, and is almost unique (up to some permutations of columns of  $\mathbf{U}$ ,  $\mathbf{W}$  and  $\mathbf{V}$ , or linear combinations of  $\mathbf{U}$  and  $\mathbf{V}$  columns with equal corresponding elements of  $\mathbf{W}$ ). Both  $\mathbf{U}$  and  $\mathbf{V}$  are orthogonal, so their inverse is simply their transpose (i.e.,  $\mathbf{U}^T \cdot \mathbf{U} = \mathbf{V}^T \cdot \mathbf{V} = \mathbf{I}$ , the identity matrix). The number of non-zero diagonal elements of  $\mathbf{W}$  (called *singular values*) gives the rank of  $\mathbf{A}$ , whereas  $\mathbf{U}$  and  $\mathbf{V}$  each contain a set of independent vectors (also called “orthonormal basis”) that fully characterize the range and null space of  $\mathbf{A}$ , respectively. Of particular interest is that the columns of  $\mathbf{V}$  whose same-numbered elements of  $\mathbf{W}$  are zero form an orthonormal basis for the null space, thus directly giving coefficients for any linear dependencies in  $\mathbf{A}$ . These, or any linear combination thereof, fully represent the range of linear relations (such as reactions or mass-balances) implicit in a matrix of compositions. A major advantage of SVD is that it allows robust handling of linear systems of equations such as Eq. (1) because of its ability to diagnose problems when the matrix of com-

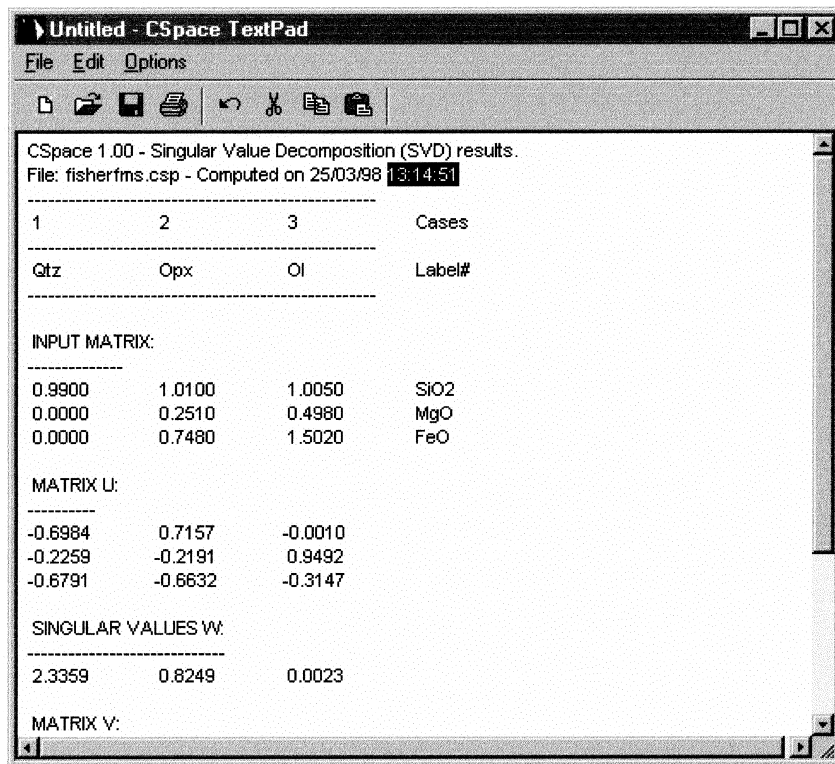


Fig. 3. TextPad window, where results from matrix routines and Matrix Analysis Wizard are written. TextPad allows editing, saving or transferring results, as appropriate.

positions  $\mathbf{A}$  is nearly singular through simple inspection of its singular values. Further, SVD also allows approximating nearly singular matrices with a nearest singular model by reversely computing Eq. (2) after replacing the smaller  $\mathbf{W}_j$ s by zero. These important subjects are discussed in the next section. The mathematics and computation of SVD are discussed by, e.g., Golub and Van Loan (1983) and Press et al. (1989).

### 3.2. SVD zero threshold and matrix modeling

From the definition of the SVD it follows that the inverse of matrix  $\mathbf{A}$  is given by

$$\mathbf{A}^{-1} = \mathbf{V} \cdot \text{diag}(1/\mathbf{W}_j) \cdot \mathbf{U}^T \quad (3)$$

(where  $\mathbf{U}^T$  refers to the transpose of  $\mathbf{U}$ ), which can be computed inasmuch as no  $\mathbf{W}_j$  is zero. If there are any  $\mathbf{W}_j$  zero values then  $\mathbf{A}$  is singular (rank-deficient) and contains as many linear dependencies. Numerically, however, ascertaining whether a matrix is singular may be compounded by computational roundoff and, more important in practice, by uncertainties in the values of the elements of  $\mathbf{A}$ . This often results in some of the computed  $\mathbf{W}_j$ s being small or very small instead of zero, effectively masking singularities as a consequence of the “noise” introduced by analytical or other errors associated to the way in which compositions were estimated.

Appropriately deciding at what threshold a small singular value should be regarded as zero is thus essential for estimating the rank of a matrix and related algebraic procedures that are based on SVD. Having the opportunity to decide on this matter, on the other hand, is one of the main advantages of using SVD with regard to other techniques such as LU decomposition or Gaussian elimination. The mapping engine of CSpace, for instance, computes the inverse of the given transformation matrix through its SVD by means of Eq. (3) and can automatically replace  $1/\mathbf{W}_j$  by zero whenever  $\mathbf{W}_j$  is zero or small enough as to be regarded as zero. In doing this, the mapping engine can diagnose and eliminate constraints that are useless or almost useless in computing the desired new coordinates.

CSpace’s algebraic tools manage the SVD zero threshold at two levels, referred to as *computational* (or default) and *user-specified*. At the computational level the tools always estimate a numeric zero threshold that is based on the ratio of the largest to the smallest singular value and the number of operations required to compute the SVD of the working matrix. This computational zero threshold (typically a very small number, often smaller than  $1e-10$ ) is appropriate for filtering out spurious non-zero singular values resulting

from roundoff errors, and should not need to be overridden when working with model/theoretical compositions that have no associated uncertainties.

To adapt for data uncertainties, a (larger) zero threshold can be specified to replace the default computational estimate. What size of zero threshold should be employed (if any) depends on the extent and distribution of likely errors in the elements of the working matrix. There are several approaches to estimating a suitable zero threshold. In most instances a simple inspection of the singular values can be used as a guide, given that obviously non-zero singular values will generally be orders of magnitude larger than suspect ones. A more rigorous assessment can be based on the data uncertainties themselves, either directly through the error propagation approach described by Powell (1990), or indirectly through matrix modeling. Matrix modeling is a most intuitive method that relies on the fact that reversely computing the SVD of a matrix after replacing the smallest non-zero singular values by zero effectively results in a “model” matrix that has a correspondingly reduced rank (contains as many additional singularities) and whose elements are “nearest” in the least-squares sense (i.e. one that minimizes the sum of the squared residuals) to the original values. If the model matrix so obtained does not differ, within likely error, from the original matrix, then it is likely that the original matrix contained as many masked singularities and the model matrix can be used to inspect the linear relations (i.e., the null-reaction space) that were “hidden” in the original matrix (see Fisher, 1989, for a more thorough discussion). CSpace’s Matrix Analysis Wizard can be directed to use this technique, and includes facilities for rapid testing of different matrix models against the known or estimated uncertainties in the original data.

## 4. The mapping engine (ME)

The transformation, or mapping, of a set of compositional coordinates into another, is useful or required in solving problems that depend on how compositions are expressed (i.e., on the component set used). Petrologic applications (see Spear et al., 1982) include the re-calculation of mineral analyses in terms of phase components, rock norms, mixing problems, preparing for projective graphical analysis and the balancing of reactions. The ME is particularly suitable for applications that require the mapping of multiple compositions. Some applications, such as balancing a reaction or exploring a mixing problem, might be better handled with the MAW, which also facilitates testing different formulations or input data sets.

In a general situation, coordinate transformation involves solving a set of  $m$  linear equations and  $n$

unknowns that relate the new components to the old ones. In matrix notation this is analogous to Eq. (1) where  $\mathbf{x}$  and  $\mathbf{b}$  are column vectors containing the  $n$  new and  $m$  old coordinates, respectively, and  $\mathbf{A}$  is an  $m$  by  $n$  matrix of coefficients whose  $n$  columns define the composition of each new component in terms of the old component set. Matrix  $\mathbf{A}$  (in this instance called the transformation matrix) can be used to map any number of objects already described with the old coordinate set by changing vector  $\mathbf{b}$  and solving repeatedly for  $\mathbf{x}$ . The solution is given by:

$$\mathbf{x} = \mathbf{A}^{-1} \cdot \mathbf{b}, \quad (4)$$

so that the kind of mapping that can be obtained depends primarily on the properties of  $\mathbf{A}$ . If  $\mathbf{A}$  is square and non-singular then the system of equations is determined and has a unique exact solution. Otherwise, it may or not have exact solution(s) depending on whether vector  $\mathbf{b}$  lies in the range of  $\mathbf{A}$ . If it does, as when there are fewer equations than unknowns and/or there are any degeneracies among them, then the system is underdetermined and has multiple exact solutions, one family of them for each corresponding vector in the null space of  $\mathbf{A}$ . If  $\mathbf{b}$  does not lie in the range of  $\mathbf{A}$ , then the system of equations is incompatible and has no (exact) solution. In the latter situation, which happens when the system is overdetermined (has more independent equations than unknowns), the problem can still be handled by using least-squares minimization techniques whose goal is to find an approximate solution that best fits the constraints of all equations.

Because of its SVD-based approach, the mapping engine of CSpace is capable of handling all these mapping problems, automatically adapting to the properties of the transformation matrix that is provided by the user. To that end the ME first checks the transformation matrix and, based on a suitable zero threshold that is accepted or supplied by the user, will determine on the fly whether the system is determined, underdetermined or overdetermined, then compute  $\mathbf{A}^{-1}$  as in Eq. (3) and use it to solve repeatedly for the new requested coordinates of all compositions to be mapped using Eq. (4). The results of the mapping and the behavior of the ME will be as follows:

- If the system is determined, the ME will perform a regular mapping. For each composition that is to be mapped the exact solution vector  $\mathbf{x}$  is computed and appended to the current database as a new set of variables.
- If the system is underdetermined then the ME will issue a warning and optionally output an exact solution vector  $\mathbf{x}$  for each composition. If a solution is requested the one provided is that with smallest length  $|\mathbf{x}|^2$ . The full set of solutions can then be obtained through linear combinations of this sol-

ution and the set of independent vectors in the null space of the transformation matrix  $\mathbf{A}$ .

- If the system is overdetermined then no vector  $\mathbf{x}$  exists that can exactly solve Eq. (1). What the ME will find instead for each composition to be mapped is the vector  $\mathbf{x}'$  that best fits all constraints in the least squares sense, i.e. one that minimizes the residual  $|\mathbf{A} \cdot \mathbf{x}' - \mathbf{b}|$ , analogous to regression for  $n$  parameters (see Fisher, 1989). Mapping to a reduced set of components is one way of projecting a composition into a composition space of less dimensions (cf. Greenwood, 1968), an alternative to projection by re-normalization or condensation (see Spear, 1988, for a discussion of the different projection methods). Also, because of the least-squares constraint, overdetermined mapping is sensitive to differential weighting, which may be useful to control mapping so that some of the equations are fit preferentially, or to impose certain constraints to the solution vector (Fisher, 1993).

## 5. The matrix analysis wizard (MAW)

The MAW is a general-purpose computational tool for matrix approximation and analysis of matrix subspaces, suitable for the algebraic analysis of mineral assemblages in rocks as well as for general mixing/mass balance problems. The MAW provides a guiding interface to the techniques and procedures advocated by Fisher (1989), and provides functionality that is equivalent to that of the DOS utilities SVDMOD and MULTI by the same author. The MAW consists of a multi-page dialog (Fig. 4) that can be walked forth and back through a number of steps up to performing complete analysis of the null-reaction space of any given matrix of compositions. MAW output is written to the *TextPad*, from where it can be saved or transferred to other applications including the DataSheet itself. Using the MAW is basically a four-step process, involving:

### 5.1. Building an input matrix

The first step is to build a collection of cases from the DataSheet containing the compositions (e.g. a phase assemblage or set of phase components) that is to be worked. Once this collection is built, the actual MAW input matrix will consist of the values of all currently active variables (which will be arranged into rows) pertaining to the collected cases (which will be arranged into columns). The input matrix may have up to 60 rows/columns. Assume, for example, that we have collected three datasheet cases, corresponding to

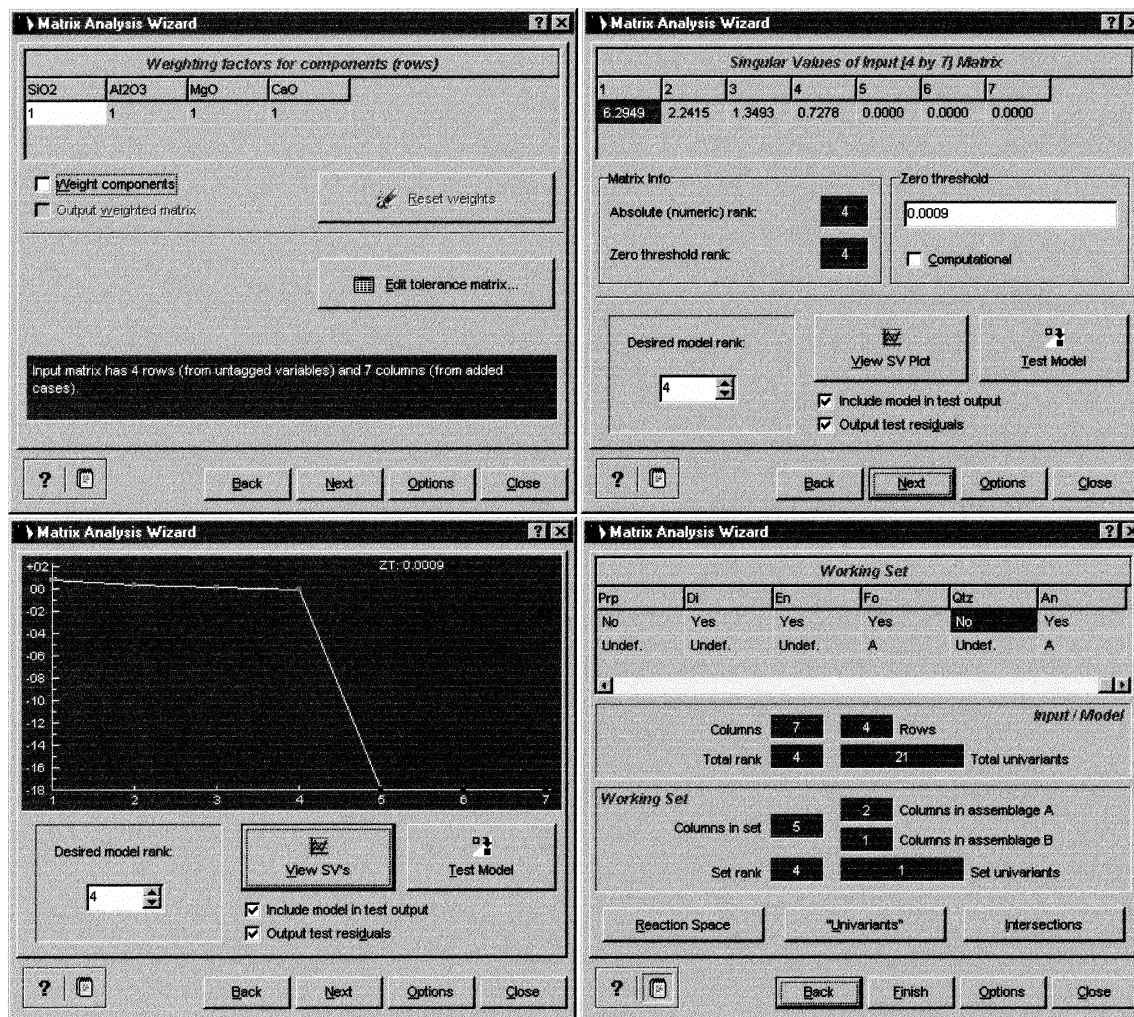


Fig. 4. Several views of pages from MAW. *Top-left*: Weights and tolerances page allows specifying whether input matrix is to be weighted and, if so, weights for each component (row). Pre-computed matrix of tolerances can also be examined and modified at this stage. *Top-right*: Modeling page displays singular values of input matrix and rank information, from which user can choose whether matrix is to be approximated by nearest rank-deficient model and, if so, test model matrix against estimated uncertainties in original data (matrix of tolerances that was specified in previous step). Test results will be output to TextPad as matrix of residual/tolerance ratios and can optionally include model matrix and residuals. *Bottom-left*: Modeling page can also display graphical plot of singular values of input matrix that includes position of currently selected zero threshold (ZT). *Bottom-right*: Last page of MAW is devoted to analysis of null (reaction) space of input/model matrix as built in preceding steps. Grid at top allows specifying what columns (i.e. phases or phase components) are to be included in computations (working set), which is useful if matrix is not model but rather matrix of theoretical phase or phase component compositions that is already rank-deficient. If problem is to find whether composition spaces of two assemblages intersect, then grid also allows specifying assemblage to which each phase belongs (either A, B or undefined). Below grid, dynamically updated information on both input/model matrix and current working set is provided, including number of selections comprising rank + 1 phases (called 'univariants'). Once all setup is done, clicking on lower row of buttons directs MAW to output desired properties of current working set, which may consist of basic vectors of null space, list of all implicit 'univariant' relationships (either complete or duplicate-filtered) and list of 'univariants' implying incompatibilities between specified assemblages (intersections).



hypothetical compositions of quartz, orthopyroxene and olivine, within the three-component system SiO<sub>2</sub>-MgO-FeMg<sub>-1</sub>. The hypothetical phase compositions were previously mapped with the ME from original SiO<sub>2</sub>-FeO-MgO molar coordinates so as to impose stoichiometric constraints on the additive components of the new set, as illustrated in Fig. 1. Upon advancing to the next MAW page, the input matrix is output to the TextPad:

1	2	3	(Case numbers)
Qtz	Opx	Ol	Label#
INPUT MATRIX:			
1.0000	1.0000	1.0000	SiO <sub>2</sub> '
0.0000	1.0000	2.0000	MgO'
0.0000	0.7485	1.5020	FeMg <sub>-1</sub>

### 5.2. Setting up component weights and tolerances

Next to building the input matrix, the user is asked to specify whether it is to be weighted and, if so, the weights to be applied to each component (Fig. 4, top-left). Weights can be specified to adjust for analytical uncertainties and/or to impose stoichiometric constraints if the matrix is to be approximated by a nearest, rank-deficient model. Weighting is optional and is limited to components (matrix rows). Although more rigorous weighting based on the full set of matrix uncertainties is theoretically required for best matrix approximation, the ways to do it are yet under research and may not be essential in practice (e.g., Powell, 1990; Lang, 1991; Whitney et al., 1995). At this stage the user can also customize the default matrix of tolerance values that has already been computed by the MAW based on the actual data in the input matrix. The matrix of tolerances is a matrix of the estimated absolute uncertainties in the original data, and is used to compute the matrix of residual/tolerance ratios when testing model matrices in the next step.

### 5.3. Matrix modeling

After having completed all the input, the user is presented with summary information on the current matrix, including its complete array of singular values and rank estimates based on the computational and user-specified zero thresholds (Fig. 4, top-right). The same information is also written to the TextPad, as in the following example, which continues developing the example matrix (data from Fisher, 1993). Note that, to keep constraining stoichiometry of additive components and force errors on the exchange component,

the former were weighted one hundred times as compared with the latter.

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\*\*\*\*ROW WEIGHTING IS ENABLED  
 \*\* New weights are in effect.

Current Row Weights:  
 100.0000            100.0000    1.0000

MATRIX U:  
 -0.5847   0.8113   0.0000  
 -0.8112   -0.5847   0.0075  
 -0.0061   -0.0044   -1.0000

SINGULAR VALUES [W]:  
 267.6293   91.5281   0.0020

MATRIX V:  
 -0.2185   0.8863   -0.4082  
 -0.5216   0.2475   0.8165  
 -0.8247   -0.3913   -0.4082

Absolute rank of Input Matrix is 3 (up to a computational zero threshold of 8.02887836168743160E-12).  
 Possible rank of Input Matrix is 3 (up to specified zero threshold: 0.0009).

---

Based on this information (which includes a graphical display of singular values; Fig. 4, bottom-left), the user may decide whether searching for a model matrix of lower rank is appropriate and, if so, test models against the original input matrix. Testing involves a comparison of both matrices, and evaluating the residuals in terms of the estimated uncertainties in the original data (i.e. the matrix of tolerances). Most useful for this purpose is the matrix of residual/tolerance ratios, which is computed as  $[(M_{ij} - A_{ij})/T_{ij}]$ , where **A** is the input matrix, **M** the model matrix being tested and **T** the matrix of tolerances that was computed or supplied in the previous step. An example test output for a suitable model matrix of rank 2 obtained from the above input matrix is as follows:

---

TEST: Model matrix of rank 2

Model matrix:

Qtz	Opx	Ol	Label#
1.0000	1.0000	1.0000	SiO <sub>2</sub> '
0.0000	1.0000	2.0000	MgO'
-0.0008	0.7502	1.5012	FeMg <sub>-1</sub>

Matrix of residuals (Model-Input):

Qtz	Opx	OI	Label#
0.0000	0.0000	0.0000	SiO2'
0.0000	0.0000	0.0000	MgO'
-0.0008	0.0017	-0.0008	FeMg <sub>-1</sub>

Matrix of residual/tolerance ratios:

Qtz	Opx	OI	Label#
0.0000	0.0000	0.0000	SiO2'
0.0001	0.0000	0.0000	MgO'
-0.8333	0.0742	-0.0185	FeMg <sub>-1</sub>

#### 5.4. Inspection of matrix relationships

Once an input/model matrix has been accepted, and provided that it contains a null (or reaction) space, the MAW will allow proceeding to its last page (Fig. 4, bottom-right), where the user can inspect the corresponding properties, either as a whole or for any working subset of matrix columns in the situation of matrices that are not models (e.g., matrices of phase components that are already rank-deficient). In each instance, the MAW can find and display the set of linearly independent basis vectors characterizing the null space in the form of linear equations among compositions (matrix columns), as well as report all or the unique (i.e. duplicate-filtered) set of “univariant” linear relationships (that is, linear relationships among phase subsets each containing rank + 1 phases) that is implicit in this reaction space. For the model matrix of rank 2 in the previous step, output of “univariants” would be as follows:

---

“UNIVARIANT” RELATIONS (null/reaction space of rank + 1 column selections)

Matrix is a working set of 3 columns out of 3 in the current input model.

Working Set:

(Working set is derived from weighted input)

Qtz	Opx	OI	
1.0000	1.0000	1.0000	SiO2'
0.0000	1.0000	2.0000	MgO'
-0.0008	0.7502	1.5012	FeMg <sub>-1</sub>

Rank of Working Set is: 2

Working Set contains 1 rank + 1 column selections (“univariants”)

“Univariant” relation(s): (unfiltered)

Qtz	Opx	OI	
[ ]			
1.0000	-2.0000	1.0000	1.0000 Qtz + 1.0000 OI = 2.0000 Opx

---

Note that the previous simplified description and example cannot fully illustrate the MAW capabilities and range of applications. For matrices that describe theoretical phases or phase components, for instance, the MAW can be easily directed to find univariant relations around any invariant (sub)assemblage or among a set of phase components. If the matrix is defined as a composite of two assemblages, the MAW can also search for “univariant” relationships between them, to see whether their composition spaces intersect (see an actual example in Table 1). For additional discussion on the procedures the reader is referred to George Fisher’s papers, as well as to actual research examples using SVD techniques (e.g., Gordon et al., 1991; Lang, 1991; Whitney et al., 1995). Additional details on MAW usage are also provided in the on-line documentation.

#### Composition diagrams

CSPACE’s graph engine is capable of generating triangular and 3D single and stereoscopic tetrahedral barycentric plots (in the latter example using a slightly modified implementation of the tetrahedral to 3D-cartesian coordinate transformation algorithm described by Spear, 1980), and includes a number of conveniences that should greatly facilitate their use for both analysis and illustration. The main features are as follows:

- The graph engine is dynamically linked to the DataSheet, and can be easily directed to use any set of variables contained therein. The DataSheet is fully functional during plotting, and any changes in the data are immediately reflected in the display. Up to 5000 cases can be plotted, and cases can be excluded or included from the plots at any time, either manually or based on the contents of any variable.
- The appearance of the diagrams can be customized interactively with regard to what is plotted (diagram outline, points, point and apex labels, tie lines), as well as to what line styles or label fonts are to be used. Re-sizing and or rotating (in the example of the 3D plots) is also done interactively either through the keyboard or by directly dragging with the mouse.
- The way points are drawn (symbol, color, size) is customizable both for a global default and individually, in the latter situation by means of suitable ‘utility variables’ that are also stored in the DataSheet. The contents of any variable (including numeric variables) can be used to label points.
- The handling of barycentric coordinates includes commutable on-the-fly scaling, Z-ordered rendering (for the 3D diagrams), and negative projection (for

Table 1  
Composition matrix, associated SVD data, reaction space, and assemblage-incompatibility relations for sample T348, cordierite-bearing pelitic gneiss from Torrox unit (Betic Belt, see García-Casco & Torres-Roldán, 1996). Table content was assembled from actual output from MAW

Composition matrix (atoms p.f.u.)													
Reactant assemblage (A)						Product assemblage (B)						Undefined	
St	Grt rim	high-Ca	Bt	Ms	PI	Rt	Crd after St	Bt	Ms	PI	Ilm after St	H <sub>2</sub> O	Qtz
			(A) matrix	(A) high-Si	(A) porph.		(B) high-Ti	(B) low-Si	(B) matrix				
Si	7.595	2.991	5.406	6.562	2.816	0.000	5.013	5.394	6.125	2.641	0.000	0.000	1.000
Al	17.935	1.970	3.601	4.783	1.187	0.000	3.980	3.434	5.707	1.353	0.000	0.000	0.000
Ti	0.136	0.006	0.304	0.118	0.000	1.000	0.001	0.524	0.050	0.000	2.015	0.000	0.000
Fe	2.974	1.875	2.701	0.223	0.000	0.000	0.880	2.685	0.094	0.000	1.874	0.000	0.000
Mn	0.062	0.023	0.022	0.003	0.000	0.000	0.029	0.016	0.001	0.000	0.097	0.000	0.000
Mg	0.505	0.625	1.608	0.376	0.000	0.000	1.048	1.463	0.075	0.000	0.000	0.000	0.000
Ca	0.000	0.528	0.001	0.000	0.200	0.000	0.004	0.001	0.003	0.380	0.000	0.000	0.000
Na	0.000	0.000	0.074	0.082	0.747	0.000	0.073	0.059	0.140	0.598	0.000	0.000	0.000
K	0.000	0.000	1.597	1.620	0.027	0.000	0.003	1.622	1.692	0.015	0.000	0.000	0.000
H	3.829	0.000	4.000	4.000	0.000	0.000	1.400	4.000	4.000	0.000	0.000	2.000	0.000

SVD data of working set (SINGULAR VALUES [W], diagonal elements):													
26.650	8.108	4.066	3.628	1.962	0.928	0.805	0.553	0.274	0.000	0.028	0.000	0.000	0.000
Absolute rank of Input Matrix is 10 (up to a computational zero threshold of 3.46450650368140267E-16).													
Possible rank of Input Matrix is 10 (up to specified zero threshold: 0.0009).													

Independent reaction set (basis vectors for the null space):												
St (A)	Grt (A)	Bt (A)	Ms (A)	PI (A)	Rt (A)	Crd (B)	Bt (B)	Ms (B)	PI (B)	Ilm (B)	H <sub>2</sub> O	Qtz
0.075	-0.154	0.187	0.571	-0.201	-0.069	-0.203	-0.137	-0.591	0.326	0.019	-0.061	0.212
0.000	-0.055	-0.604	0.189	-0.074	-0.192	0.075	0.594	-0.180	0.115	0.025	-0.050	-0.385
0.000	-0.214	-0.071	-0.374	-0.438	-0.098	0.065	0.207	0.228	0.526	0.022	-0.028	0.480

Assemblage incompatibilities (found 13 assemblage incompatibilities out of 78 possible reactions involving rank + 1 phases):												
St (A)	Grt (A)	Bt (A)	Ms (A)	PI (A)	Rt (A)	Crd (B)	Bt (B)	Ms (B)	PI (B)	Ilm (B)	H <sub>2</sub> O	Qtz
0.000	10.783	0.000	20.529	22.278	3.912	-2.922	-7.126	-12.940	-26.554	-1.000	1.119	-27.228
0.000	34.448	101.660	16.328	64.589	41.412	-19.493	-116.689	0.000	-81.599	-6.594	11.047	1.000
0.000	73.320	213.916	35.944	137.632	87.443	-41.244	-246.091	-1.000	-173.755	-13.953	23.333	0.000
7.508	0.000	183.716	6.441	1.000	45.599	-40.916	-176.332	-10.481	0.000	-5.097	7.581	125.159
-3.344	0.000	-13.936	-35.759	-4.843	-1.000	11.440	15.815	32.270	2.160	0.000	1.613	3.012
4.555	0.000	48.891	34.227	4.660	9.868	-18.573	-49.174	-31.803	-1.991	-1.000	0.000	21.779
28.730	0.000	149.655	292.778	39.673	17.099	-101.288	-163.523	-265.130	-17.605	-1.000	-11.666	0.000

(continued on next page)

Table 1 (continued)

Composition matrix (atoms p.f.u.)		Product assemblage (B)										Undefined	
Reactant assemblage (A)		Product assemblage (B)										Undefined	
St	Grt rim high-Ca	Bt (A) matrix	Ms (A) high-Si	Pl (A) porph.	Rt	Crd after St	Bt (B) high-Ti	Ms (B) low-Si	Pl (B) matrix	Ilm after St	H <sub>2</sub> O	Qtz	
11.463	28.011	0.000	199.082	77.571	0.000	-42.040	-28.591	-163.682	-77.904	-1.000	-6.137	-122.413	
-1.768	-13.440	0.000	-48.068	-30.806	-3.308	8.956	10.437	36.189	34.473	1.000	0.000	41.909	
1.000	1.700	32.919	0.000	3.098	9.093	-6.755	-32.416	0.000	-3.917	-1.119	1.807	19.691	
-41.501	-1.000	-1092.955	0.000	-2.580	-274.440	234.183	1046.909	27.660	0.000	30.856	-47.697	-756.327	
1.809	1.270	4.018	23.471	5.472	0.000	-6.182	-6.142	-20.416	-4.408	0.000	-1.000	-7.885	
-3.602	-4.596	-32.172	-38.960	-13.601	-7.625	15.284	35.927	33.303	13.099	1.000	0.000	0.000	

Actual reactions (coefficients normalized to smallest non-zero value):

10.78 Grt + 20.52 Ms(A) + 22.27 Pl(A) + 3.91 Rt + 1.12 H<sub>2</sub>O = 2.92 Crd + 7.13 Br(B) + 12.94 Ms(B) + 26.55 Pl(B) + 1.00 Ilm + 27.23 Qtz

34.45 Grt + 101.66 Br(A) + 16.33 Ms(A) + 64.59 Pl(A) + 41.41 Rt + 11.05 H<sub>2</sub>O + 1.00 Qtz = 19.49 Crd + 116.69 Br(B) + 81.60 Pl(B) + 6.59 Ilm

73.32 Grt + 213.92 Br(A) + 35.94 Ms(A) + 137.63 Pl(A) + 87.44 Rt + 23.33 H<sub>2</sub>O = 41.24 Crd + 246.09 Br(B) + 1.00 Ms(B) + 173.75 Pl(B) + 13.95 Ilm

7.51 St + 183.72 Br(A) + 6.44 Ms(A) + 1.00 Pl(A) + 45.60 Rt + 7.58 H<sub>2</sub>O + 125.16 Qtz = 40.92 Crd + 176.33 Br(B) + 10.48 Ms(B) + 5.10 Ilm

11.44 Crd + 15.81 Br(B) + 32.27 Ms(B) + 2.16 Pl(B) + 1.61 H<sub>2</sub>O + 3.01 Qtz = 3.34 St + 13.94 Br(A) + 35.76 Ms(A) + 4.84 Pl(A) + 1.00 Rt

4.55 St + 48.89 Br(A) + 34.23 Ms(A) + 4.66 Pl(A) + 9.87 Rt + 21.78 Qtz = 18.57 Crd + 49.17 Br(B) + 31.80 Ms(B) + 1.99 Pl(B) + 1.00 Ilm

28.73 St + 149.65 Br(A) + 292.78 Ms(A) + 39.67 Pl(A) + 17.10 Rt = 101.29 Crd + 163.52 Br(B) + 265.13 Ms(B) + 17.60 Pl(B) + 1.00 Ilm + 11.67 H<sub>2</sub>O

11.46 St + 28.01 Grt + 199.08 Ms(A) + 77.57 Pl(A) = 42.04 Crd + 28.59 Br(B) + 163.68 Ms(B) + 77.90 Pl(B) + 1.00 Ilm + 6.14 H<sub>2</sub>O + 122.41 Qtz

8.96 Crd + 10.44 Br(B) + 36.19 Ms(B) + 34.47 Pl(B) + 1.00 Ilm + 41.91 Qtz = 1.77 St + 13.44 Grt + 48.07 Ms(A) + 30.81 Pl(A) + 3.31 Rt

1.00 St + 1.70 Grt + 32.92 Br(A) + 3.10 Pl(A) + 9.09 Rt + 1.81 H<sub>2</sub>O + 19.69 Qtz = 6.75 Crd + 32.42 Br(B) + 3.92 Pl(B) + 1.12 Ilm

234.18 Crd + 1046.91 Br(B) + 27.66 Ms(B) + 30.86 Ilm = 41.50 St + 1.00 Grt + 1092.96 Br(A) + 2.58 Pl(A) + 274.44 Rt + 47.70 H<sub>2</sub>O + 756.33 Qtz

1.81 St + 1.27 Grt + 4.02 Br(A) + 23.47 Ms(A) + 5.47 Pl(A) = 6.18 Crd + 6.14 Br(B) + 20.42 Ms(B) + 4.41 Pl(B) + 1.00 H<sub>2</sub>O + 7.88 Qtz

15.28 Crd + 35.93 Br(B) + 33.30 Ms(B) + 13.10 Pl(B) + 1.00 Ilm = 3.60 St + 4.60 Grt + 32.17 Br(A) + 38.96 Ms(A) + 13.60 Pl(A) + 7.62 Rt

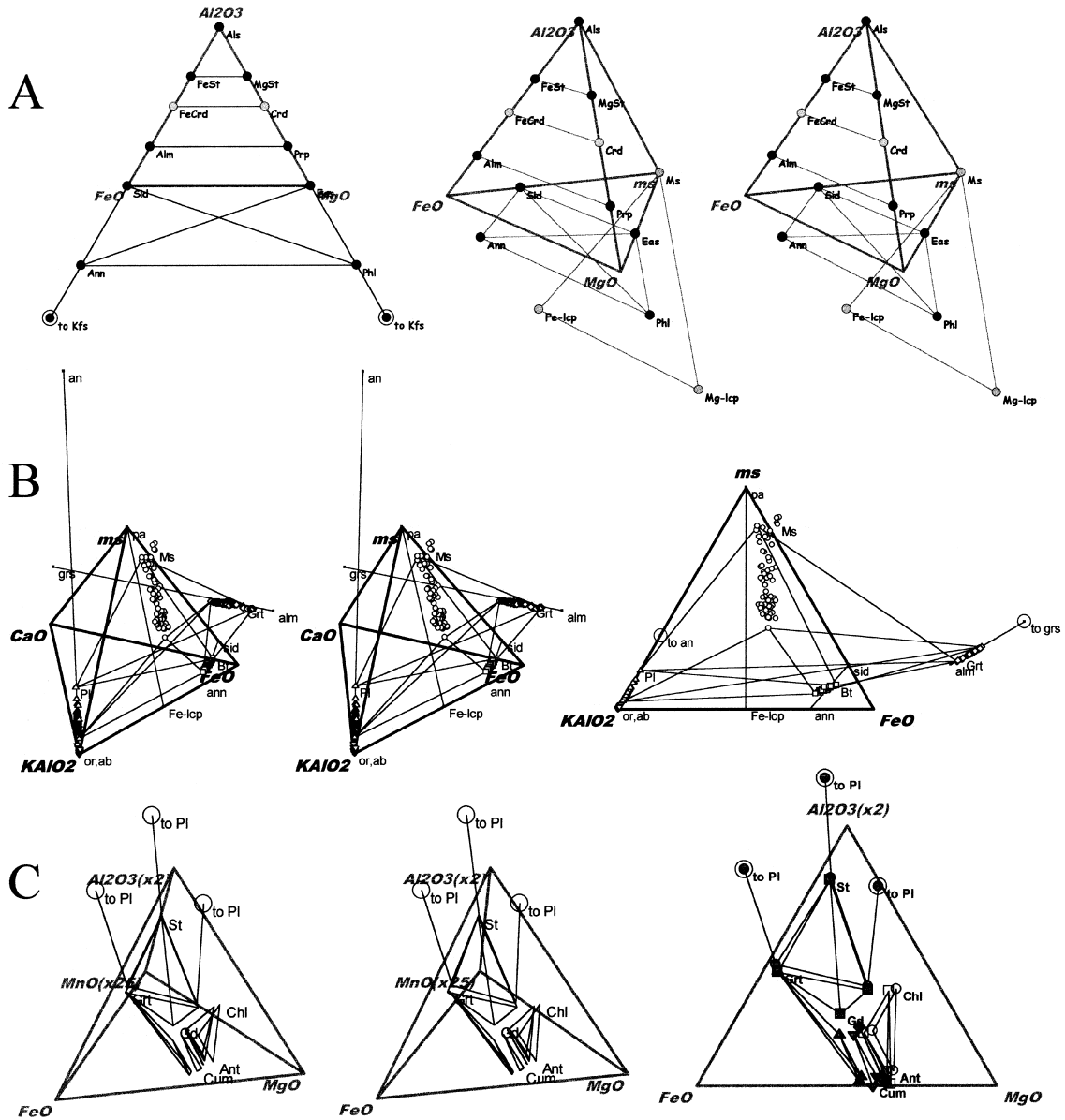


Fig. 5. Examples of compositional barycentric plots generated by CSpace. (A) Right: stereoscopic view of Muscovite(Ms)-FeO-MgO- $Al_2O_3$  tetrahedron, projected from quartz and  $H_2O$ , with projection of Al-silicate, K-feldspar and representative end-members of muscovite, biotite, garnet, staurolite and cordierite. Left: same elements as projected additionally from muscovite onto FeO-MgO- $Al_2O_3$  plane. Note that K-feldspar does not find projection in tetrahedral diagram, but can be linked in ternary plot to any existing phase by means of tie-line connection through infinity (to biotite in example). Leucophyllite components, on other hand, do not find projection in ternary diagram. (B) Phase relationships in high-grade  $Ms + Bt + Grt + Kfs + Pl$  gneisses from Torrox Gneiss Complex (García-Casco et al., 1993) plotted in  $KAlO_2$ - $CaO$ - $FeO$ - $MgO$  tetrahedron (projected from rutile, quartz,  $H_2O$  and exchange vectors  $KNa_{-1}$ ,  $MgFe_{-1}$  and  $MnFe_{-1}$ ) and in  $KAlO_2$ - $FeO$ - $MgO$  triangle (projection points as before, in addition to  $CaO$ ). Two sets of tie lines represent high-P and low-P assemblages (both Kfs-bearing, which plots close to  $KAlO_2$  apex). Also plotted are representative end members of phases of interest, joined with lines to illustrate nature of compositional variations. Note that components anorthite and grossular plot through infinity in triangular plot. (C) Phase relationships in carbonate-absent amphibolites from Post Pond Volcanics, Vermont, plotted in  $Al_2O_3$ - $FeO$ - $MgO$ - $MnO$  tetrahedron in stereoscopic view (projected from quartz,  $H_2O$ ,  $Pl(an_{3.5})$  and average hornblende), and in  $Al_2O_3$ - $FeO$ - $MgO$  triangle (projection points as before, in addition to  $MnO$ ). Note that Mn has been scaled ( $\times 25$ ) in tetrahedral plot, and that plagioclase ( $an_{90}$ ) plots through infinity in both diagrams (data from Spear, 1982).

points with negative coordinate sum). ‘Negative’ points can also be handled (more appropriately) through the projection of tie lines that connect them to other ‘positive’ elements of the assemblage. Continuous feedback about the set of points intended to plot and how many of these are actually plotted is given, as well as means for investigating why some points could be missing from the plots.

- Cases may be marked as belonging to an assemblage, and this information can be used to connect them with tie lines in the diagrams. In this way up to 1000 tie line sets (each comprising up to four points) can be automatically drawn, including the ability to have each tie set rendered in a distinctive color. Handling of tie lines connecting points ‘through infinity’ is done automatically, without user intervention. Tie line sets can also be used to represent the phase region of solutions or to divide the diagram into areas of particular interest (e.g., as in diagrams used for geochemical classifications of rocks or minerals).

Fig. 5 gives some examples of diagrams produced by CSpace. All the examples represent unmodified output (except for color, that was removed to facilitate printing). The whole figure was assembled by importing individual disk metafiles exported from CSpace into a commercial graphics package.

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