Transformed major element based multidimensional classification of altered volcanic rocks

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To fill the gap of the nomenclature of altered igneous rocks, a new exhaustive multidimensional classification scheme consistent with the International Union of Geological Sciences (IUGS) is proposed. Our procedure is based on an extensive database of major element compositions of a total of 32948 relatively fresh rock samples. The database consisted of multinormally distributed samples in terms of their 9 isometric log-ratios. The set of 48 new diagrams along with 76 discriminant functions provided acceptable success rates for most of the 17 root-names and 10 additional sub-root names. A new computer program IgRoClaMSys_ilr was written to facilitate an efficient use of our proposal. Good functioning of our multidimensional procedure was ascertained from 4 test studies of relatively fresh rocks, whereas 5 application studies of altered igneous rocks showed, as expected, greater discrepancy between the new and the IUGS schemes. Another important and novel application of this scheme for inferring the rock type of igneous provenance of siliciclastic sediments was demonstrated through 3 further application studies. IgRoClaMSys_ilr is also equipped with modules for ascertaining robustness of the new scheme with respect to analytical errors and post-emplacement compositional changes, including those related to hydrothermal alteration and low-grade metamorphism.

Introduction

According to the International Union of Geological Sciences (IUGS), the volcanic rocks can be classified from the well-known TAS (total alkalis versus silica) diagram after the separation of high-Mg rocks (Le Bas et al., 1986; Middlemost, 1994; Le Bas, 2000; Le Maitre et al., 2002). It is also clear that the TAS scheme proposed for 17 root names and 10 more sub-root names (Le Bas et al., 1986) should not be used for the classification of altered rocks. Le Bas et al. (1986) made the following points clear in their IUGS proposal (only some salient features are reproduced): (i) “The classification is purely descriptive” and “no genetic relationships are implied”; (ii) “It was designed for unaltered volcanic rocks”, however, Middlemost (1994) has proposed a similar scheme for plutonic rocks; and (iii) “Analyses with $H_2O > 2$ weight per cent or with $CO_2 > 0.5$ per cent should be regarded with suspicion. All analyses must be recalculated to 100 per cent and free of $H_2O$ and $CO_2$”.

The IUGS classification will not be suitable for metamorphic rocks involving post-emplacement chemical changes. For altered rocks, the IUGS did not recommend any classification procedure (Le Bas et al., 1986; Le Maitre et al., 2002). The available schemes, such as Floyd and Winchester (1975, 1978) Winchester and Floyd (1976, 1977), have been shown unsuitable for this purpose (Verma et al., 2010).

The chemical compositions of altered rocks can be considerably modified from their initial concentrations. This includes SiO$_2$ and total alkalis (Na$_2$O and K$_2$O) as well. Besides, the compositional data per se are characterized by a constant sum and closure problem (e.g., Chayes, 1960; 1978; Butler, 1979, 1982) and certain statistically coherent solutions are required (e.g., Aitchison, 1984, 1986, 1999; Egozcue et al., 2003; Verma, 2015). The constant sum also renders that concentrations of all elements, whether mobile or immobile, will change if the rock is altered after its emplacement (Verma, 2015; Verma et al., 2016a, 2017a).

The IUGS has recommended that the classification of plutonic rocks be achieved through minenological considerations (e.g., Streckeisen, 1966, 1967; Le Bas et al., 1986; Le Maitre et al., 2002). However, there are certain well documented problems with the use of ternary diagrams (Butler, 1979; Verma, 2012, 2015). Nevertheless, the use of chemical classification for plutonic rocks consistent with the TAS scheme was suggested by Middlemost (1994). Such a classification will be especially useful when precise modal compositions are not available, being the case of most modern geochemical studies. However, this classification scheme meant for fresh rocks will not be applicable to altered rocks.

We propose a statistically coherent solution to the problem of altered rock nomenclature in terms of all 17 root-names and 10 additional sub-root names for volcanic and plutonic rocks in the multidimensional space of all major element log-ratios. The new multidimensional...
scheme is evaluated from fresh igneous rocks not included in the original database and its application to altered volcanic or plutonic rocks is suggested as an essential step towards an adequate classification. The post-emplacement changes may be due to hydrothermal alteration or low-grade metamorphism. A novel application is also documented for deciphering the rock type of igneous provenance of siliciclastic sediments.

Methods

Database

A worldwide representative database of major element compositions of relatively fresh Neogene igneous rocks was established. A total of 32948 samples with their schematic locations in Figure 1 are summarized in Table S1 (see Supplementary data file available for downloading from the journal website, as well as from our website tlaloc.ier.unam.mx). The samples compiled from over 1000 papers were first classified from the IUGS scheme applied through the IgRoCS computer program (Verma and Rivera-Gómez, 2013). A synthesis of the complete database is available from http://tlaloc.ier.unam.mx/index.html.

For the proposal of the new scheme, major elements were adjusted to 100% on an anhydrous basis with total Fe as Fe$_2$O$_3$ from equations listed in Table S2. The conversion to Fe$_2$O$_3$ was achieved from the first equation in Table S2. This equation will be useful, irrespective of whether Fe was reported as FeO or as its two oxidation varieties FeO and Fe$_2$O$_3$. The use of FeO instead of Fe$_2$O$_3$ for the proposal of our multivariate classification technique will not change the conclusions; only the coefficients of the discriminant function equations will change. The major element adjusted data were then transformed to isometric log-ratios from equations of Table S3. The conversion of Fe and later adjustment to 100% anhydrous, render the database more uniform and suitable for their log-ratio transformation.

Log-ratio Transformation and Multinormality Tests

Isometric log-ratio (ilr) transformation of Egozcue et al. (2003) was used. The other transformations (additive and centred log-ratios of Aitchison, 1986) would provide the same final results for any given database (Verma, 2015). The multinormality test (Wilks, 1963; Barnett and Lewis, 1994; Rencher, 2002) was applied through a new computer program DOMuDaF by Verma et al. (2016a), which has also been successfully used by Verma et al. (2017a) for inferring discordancy of multivariate outliers and proposing a new magma type classification scheme. Thus, only the multinormally distributed samples in terms of their 9 log-ratios were considered.

Linear Discriminant and Canonical Analysis

The multinormally distributed ilr data of 32948 samples were used for the application of the multivariate technique of linear discriminant analysis (LDA) and canonical analysis (Table S1; the individual transformed data are not shown here but will be available as Excel files from http://tlaloc.ier.unam.mx/index.html). The tests for equality of group means show that all 9 log-ratios (ilr1TiM to ilr9PM) have statistically significant differences among the four main classes or groups of magma types at a low significance level approaching 0.000000 (Table S4). All ratios can therefore be used for further analysis. Similarly significant differences were also observed for different rock types but are not reported here to keep the paper short.

The complete database of multinormally distributed isometric log-ratios of 32948 (1505 ultrabasic, 12204 basic, 11750 intermediate and 7489 acid; Table S1) rock samples was used for proposing a set of 48 new diagrams (only a few diagrams are shown in the Supplementary data file) and 76 discriminant functions (all equations are listed in the Supplementary data file). After carrying out LDA, probabilities for individual samples were calculated from the method outlined by
Agrawal (1999), Verma and Agrawal (2011) or Verma and Verma (2013). They were used in this work to decide the classification field in which a given sample will plot. For probability calculations, group centroids represented by the mean values were used, because this statistical parameter would provide the best estimate of the central tendency when appropriate discordancy tests are used for identifying and separating discordant outliers from the datasets (Verma et al., 2016b, 2017b).

**Computer Program for Classification for Altered Igneous Rocks**

For an efficient application of the new multidimensional scheme, a computer program IgRoClaMSys_ilr (Igneous Rock Classification Major-element based System from isometric log-ratios) was written in Java Framework ZK (Fig. 2). Before using the program, the user must make sure that the rocks to be processed in IgRoClaMSys_ilr are not of high-Mg type (Le Bas, 2000). For such fresh rocks, the original criteria (Le Bas, 2000) can be used but, for altered rocks, it may be necessary to first use a published computer program HMgClaMSys_mlr (Verma et al., 2016a; usable at http://tlaloc.ier.unam.mx/index.html) in order to ascertain the high-Mg nature of altered rocks. If the rocks are classified as of high-Mg type, HMgClaMSys_mlr will provide their nomenclature (komatiite, meimechite, picrite, and boninite), consistent with the IUGS (Le Bas, 2000).

The first part of IgRoClaMSys_ilr concerns data validation and transformation (Tables S2 and S3). The information on whether one is

![Figure 2. Schematic flow diagram of the new computer program IgRoClaMSys_ilr. The abbreviations used are as follows: U – ultrabasic; B – basic; I – intermediate; A – acid; BSN – basanite; TEP – tephrite; PB – picrobasalt; FOI – foidite; BSN, bsn – basanite, basanite; BSN, mnp – basanite, melanephelinite; BSN, np – basanite, nephelinite; TEP, bsn – tephrite, basanite; TEP, mnp–tephrite, melanephelinite; TEP, np – tephrite, nephelinite; FOI, bsn – foidite, basanite; FOI, mnp – foidite, melanephelinite; FOI, np – foidite, nephelinite; B – basalt; TB – trachybasalt; BsnTepFoi – group of basic basanite, tephrite, and foidite; BtaPhtTphPh – group of basaltic trachyandesite, phonotephrite, tephriphonolite, and phonolite; B, alk – basalt, alkali; B, subalk – basalt, subalkali; TB, haw – trachybasalt, hawaiite; TB, pot – trachybasalt, potassic; BA – basaltic andesite; A – andesite; BtaTAT – group of basaltic trachyandesite, trachyandesite, and trachyte; BtaPhtTphPh – group of basaltic trachyandesite, phonotephrite, tephriphonolite, and phonolite; Bta, mug – basaltic trachyandesite, mugearite; Bta, sho – basaltic trachyandesite, shoshonite; TA, ben – trachyandesite, benmoreite; TA, lat – trachyandesite, latite; T, palk – trachyte, peralkaline; D – dacite; TD – trachydacite; T – trachyte; R – rhyolite; T, palk – trachyte, peralkaline; R palk – rhyolite, peralkaline.](image)
New Multidimensional Scheme

The complete database was subdivided into four magma types, for which 10 multidimensional discriminant functions (Eqs. S1 to S10 in Table S5) in 5 DF1-DF2 type diagrams (Figs. S1a–e) were proposed. The probability-based boundary coordinates in these five diagrams are listed in Table S6. The percent success in these diagrams (Figs. S1a–e) varied from 79.3% to 99.3% (Table S7). One sample (ME90-11; Binard et al., 1993) was used to illustrate the procedure. According to the IUGS scheme, this is an ultrabasic rock; the data are plotted in Figures S1a–e (filled diamond) and the respective probability values are summarized in Table S8. The final synthesis of percent probability (%prob of 70.8%; Table S8) from the new scheme clearly confirmed that this is an ultrabasic rock. Because a given field is always absent in any set of such diagrams (Figs. S1a–e), the final percent probability for any given field can never reach 100%. The overall percent success (correct classification as a synthesis of all five diagrams; Figs. S1a–e) varied from 79.3% to 99.3% (Table S7). One sample (ME90-11; Binard et al., 1993) was used to illustrate the procedure. According to the IUGS scheme, this is an ultrabasic rock; the data are plotted in Figures S1a–e (filled diamond) and the respective probability values are summarized in Table S8. The final synthesis of percent probability (%prob of 70.8%; Table S8) from the new scheme clearly confirmed that this is an ultrabasic rock. Because a given field is always absent in any set of such diagrams (Figs. S1a–e), the final percent probability for any given field can never reach 100%. The overall percent success (correct classification as a synthesis of all five diagrams; Figs. S1a–e) varied from 79.3% to 99.3% (Table S7).

Basalt can be subdivided into its two varieties (alkali and subalkali basalts) from the discriminant function (Eq. S37 in Table S25). The percent success for this rock type was high (95.7% for alkali basalt and 91.4% for subalkali basalt; Table S26). Similarly, trachybasalt was subdivided as hawaiite and potassic varieties (discriminant function Eq. S38; Table S27). The success values for this subdivision were also high (94.2% for hawaiite and 86.9% for potassic variety or sub-root name; Table S28).

The group BsnTepFoi was separated into three rock types (basanite, tephrite, and foidite) from the discriminant function Equations (S39) and (S40) (Table S29). The probability-based boundary coordinates are listed in Table S30. The percent success values for this three-fold division varied from 84.3% to 95.1% (Table S31). Using Equations (S41) and (S42) (Table S32), the basanite was further subdivided into three sub-varieties (basanite, melanephelinite, and nephelinite). Similarly, tephrite was subdivided into the same three sub-varieties from Equations (S43) and (S44) (Table S33) and foidite into two sub-varieties (melanephelinite and nephelinite) from Equation (S45) (Table S34). The boundary coordinates for the basanite and tephrite subdivision are listed in Table S35. The percent success values ranged from 87.3–93% for basanite, 84–91% for tephrite, and 100% for foidite (Table S36).

The group BtaPhtTphPh was also divided into three rock types (basaltic trachyandesite, phonotephrite, and combined tephrphonolite and phonolite) from Equations (S46) and (S47) (Table S37). The field boundaries are listed in Table S38. The percent success values varied from about 83% to 93.6% (Table S39). Basaltic trachyandesite was subdivided as two sub-varieties (mugearite and shoshonite) from Equation S48 (Table S40) with percent success of 96.4% and 88.9%, respectively (Table S41). The two rock types (tephrphonolite and phonolite) were divided into two sub-varieties from Equation (S49) (Table S42) with success values of 100% (Table S43).

The intermediate rocks were first divided as basaltic andesite (BA), andesite (A), group of basaltic trachyandesite, trachyandesite and trachyte (BtaTAT), and group of phonotephrite, tephrphonolite and phonolite (PhtTphPh). The relevant discriminant function Equations (S50) to (S59) and field boundaries are given in Tables S44 and S45, respectively. Table S46 provides the percent success values that vary from
83.5% to 95.6%, whereas Table S47 reports the overall success rates for the classification of the intermediate rocks as four rock groups which varied from 80.8% for the group of BtaTAT to 91.5% for basaltic andesite.

The intermediate rock group BtaTAT was further divided into the three rock types (basaltic trachyandesite, trachyandesite, and trachyte) from discriminant function Equations (S60) and (S61) (Table S48; boundary coordinates in Table S49) with percent success values of 85.5% to 94.8% (Table S50). The basaltic trachyandesite rocks were further subdivided for sub-root rock names of mugearite and shoshonite from Equation (S62) (Table S51), with percent success values of 98.5% and 82.9%, respectively (Table S52). Trachyandesite rocks were similarly subdivided as its two sub-root rock names of mugearite and latite (Eq. S63; Table S53) with percent success values of 97.3% and 78.9%, respectively (Table S54). The intermediate trachyte rocks were subdivided as trachyte and peralkaline trachyte from discriminant function Equation (S64) (Table S55) and percent success values of 96.2% and 90% were obtained for this subdivision (Table S56).

The intermediate rock group PhtTphPh was divided into three rock types phonotephrite (Pht), tephriphonolite (Tph), and phonolite (Ph) from Equations (S65) and (S66) (Table S57; boundary coordinates in Table S58) with percent success values listed in Table S59.

Finally, the acid rocks were first divided in five diagram set as dacite, trachydacite, trachyte, and rhyolite (Eqs. S67 to S76; Table S60; boundary coordinates in Table S61). The percent success values for individual diagrams varied from 72.9% to 98.5% (Table S62), whereas the overall success values ranged from 77.6% for trachyte to 86.9% for dacite (Table S63).

The acid trachyte rocks were subdivided as two sub-root names (trachyte and peralkaline trachyte) from Equation (S77) (Table S64) and percent success values of 95.9% and 88.9% were obtained (Table S65). Finally, rhyolites were subdivided as rhyolite and peralkaline rhyolite from Equation (S78) (Table S66) obtaining success values of 99.4% and 95.9%, respectively (Table S67).

Discussion

This section is subdivided into four subsections: (1) Overall success of the alternative IgRoClaMSys_ilr scheme for assigning root and sub-root names for the complete database evaluated in the light of the IUGS scheme as a reference; (2) Success of the new scheme for individual test studies of fresh rocks also evaluated against the IUGS scheme; (3) Application of IgRoClaMSys_ilr to altered igneous rocks evaluated against the original IUGS scheme proposed for fresh rocks only; (4) Additional application studies for igneous provenance of siliciclastic sediments; and (5) Mention of the additional modules of IgRoClaMSys_ilr for ascertaining the robustness of the new scheme with respect to analytical errors and post-emplacement compositional changes.

Overall Success for the Alternative IgRoClaMSys_ilr Scheme

The complete database (32948 analyses) was first processed to evaluate the correctness or percent success of the classification of 17 root names (Table 1) and all 29 root and sub-root names (Table S68). The IUGS scheme (Le Bas et al., 1986) was used as reference. For 12 root names, the percent success was relatively high 62.4% for tephriphonolite to 86.7% for rhyolite (Table 1). For the remaining 5 root names, it was lower, although for only two cases (picrobasalt and phonolite), it could be considered unacceptably low (Table 1). Similarly, for 29 root and sub-root names of Le Bas et al. (1986) percent success values of > 50% were obtained for 22 rock types, with the remaining rock types showing lower values (Table S68). Nevertheless, these percent success values are significantly higher than those obtained for the available alternative diagrams of Floyd and Winchester (1975, 1978) Winchester and Floyd (1976, 1977) as demonstrated by Verma et al. (2010).

Testing of the New Rock Classification Scheme from Fresh Rocks

This IgRoClaMSys_ilr scheme was then applied for testing from relatively fresh rock data not included in the initial database (Tests T1 to T4 in Fig. 1).

For the first test (T1; Fig. 1; Table S69), the data for 62 Quaternary volcanic rock samples of Kaula volcanics, Hawaiian Islands (Garcia et al., 2016) indicated from the IUGS classification that 14 rocks were ultrabasic (3 basanite, basanite; 4 basanite, melanephelinite; 4 foidite, melanephelinite; 1 foidite, nephelinite; and 2 picrobasalt) and 48 basic (40 basalt, alkali; 1 basalt, subalkali; 6 basanite, basanite; and 1 trachybasalt, hawaiite). In terms of magma types, the IgRoClaMSys_ilr scheme provided 10 ultrabasic and 52 basic rocks, thus misclassifying only 4 ultrabasic as basic rocks. Thus, 58 out of 62 magma types as correctly classified amounted to about 94% correct classification. Now, in terms of rock types, the IgRoClaMSys_ilr correctly classified 40 samples of alkali basalt; 1 subalkali basalt; 1 basanite, basanite; and 4 basanite, melanephelinite (Table S69) amounting to about 74% correct classification. The incorrect classification was mainly the “neighbour” rock types, not drastically different from the original IUGS rock types (Table S69) because 8 basanite, basanite were classified as alkali basalt; 1 foidite, nephelinite as basanite, basanite; 4 foidite, melanephelinite as basanite, melanephelinite; 2 picrobasalt as alkali basalt; and 1 trachybasalt, hawaiite as alkali basalt.

The next test (T2; Fig. 1; Table S70) was from Holocene volcanic rocks of San Antonio volcano, Tacaná volcanic complex, Mexico-Guatemala (Mora et al., 2004). Out of 14 rock samples (IUGS: 12 intermediate and 2 acid rocks), 13 were correctly classified in terms of magma types (IgRoClaMSys_ilr: 11 intermediate and 3 acid rocks). In terms of rock types, 3 basaltic andesite, 8 andesite, and 1 rhyolite were correctly classified, with only 2 rocks (1 andesite and 1 rhyolite) incorrect as dacitic rocks.

Test T3 (Fig. 1; Table S71; Di Piazza et al., 2015) included 7 Quaternary volcanic rock samples of Turrialba volcano, Costa Rica. Out of 7 intermediate rocks, 6 proved to be as such, with the remaining classified as an acid rock, whereas, in terms of rock types, 5 (3 basaltic andesite and 2 andesite) were correctly classified (Table S71). One trachyandesite, benmorite was wrongly classified as andesite and 1 andesite as trachyte.

For Test T4 (Fig. 1; Table S72; Shaw et al., 2003), 32 Miocene–Pleistocene volcanic rock samples of Harrat Ash Shaam, Jordan were compiled. From the IUGS scheme, they were classified as 9 ultrabas-
sic (8 basanite, basanite; and 1 basanite, nephelinite) and 23 basic (17 basalt, alkali; and 6 basalt, subalkali) rocks. The IgRoClaMSys_ilr identified 6 samples as ultrabasic and 26 as basic, thus correctly classifying 29 samples for their magma types (Table S72), amounting to about 90% success. In terms of rock types, 29 samples (16 alkali basalt; 6 subalkali basalt; 6 basanite, basanite; and 1 basanite, nephelinite) were correctly classified by IgRoClaMSys_ilr. Only 2 basanite, basanite were misclassified as 2 alkali basalt and 1 alkali basalt as subalkali basalt (Table S72).

Thus, all four tests clearly show that the new scheme works well for the classification of fresh rocks.

**Application to Older Igneous Rocks**

For the new IgRoClaMSys_ilr scheme to be useful for the classification of older rocks, there should be more differences or inconsistencies with the IUGS scheme put forth for fresh rocks only. We present 4 application case studies (A1 to A4; Fig. 1) to illustrate the usefulness of IgRoClaMSys_ilr.

The first application is for the Paleoproterozoic Star Lake pluton, Canada (Application study A1; Fig. 1; Janser, 1992, 1994). Out of 78 analyses, 33 intermediate and 23 acid rocks from the IUGS scheme also proved to be as such from the IgRoClaMSys_ilr (Table S73). Nine basic and 13 acid rocks were classified as intermediate rocks by the new scheme, amounting to about 28% incorrect classification of magma types. The classification of rock types was even worse because only 38 samples (out of 78; Table S73) were correctly classified, amounting to only 49% correct classification. Because the studied rocks are plutonic, the equivalent plutonic rock names are provided in the last column (Table S73).

Our next application is for Paleozoic volcanic rocks of Juchatengo Complex, Mexico (Application study A2; Fig. 2; Table S74; Grajales-Nishimura et al., 1999). Out of 13 samples classified as basic rocks from the IUGS scheme, 4 were classified as intermediate rocks from the IgRoClaMSys_ilr. Similarly, for their rock types, 5 out of 13 were differently classified by the IgRoClaMSys_ilr (Table S74).

Another application is concerned with Paleoproterozoic lava and sheeted dyke samples from Jormua ophiolite, Finland (Application study A3; Fig. 2; Table S75; Peltonen et al., 1996). Twenty-four out of 33 basic rock samples (according to the IUGS scheme) were classified as basic rocks, with the remaining 9 samples differently classified as ultrabasic (3 samples) and intermediate (6 samples). Similarly, only 21 out of 33 samples (amounting to about 64%) were classified as the same rock types by both schemes (Table S75).

Our next application is to Mesoproterozoic rocks of Delhi area, India (Application study A4; Fig. 2; Table S76; Abu-Hamatteh, 2000). From the IUGS scheme, 24 rock samples were classified as 1 ultrabasic, 13 basic, and 10 intermediate rocks, whereas from the IgRoClaMSys_ilr, the same rocks were subdivided as 2 ultrabasic, 20 basic, and 2 intermediate rocks. Similarly, The IUGS scheme determined these rocks as 1 picrobasalt, 2 alkali basalt, 11 subalkali basalt, 6 basaltic andesite, 2 basaltic trachyandesite (1 mugearite and 1 shoshonite), and 2 andesite.

### Table 1. Classification of rock types (root names) from the initial database from the new multidimensional classification scheme and comparison with the IUGS classification scheme

| Rock no. | Rock name (IUGS) | No. of samples (IUGS) | Number of samples classified from IgRoClaMSys_ilr in any given field | Percent success (IgRoClaMSys_ilr) |
|----------|------------------|-----------------------|---------------------------------------------------------------|----------------------------------|
| 1        | basanite         | 1484                  | 482 189 3 71 65 20 63                                        | 72.3                             |
| 2        | tephrite         | 312                   | 1 245 1 13 6 1 44 1                                           | 78.5                             |
| 3        | picrobasalt      | 72                    | 7 5 21 39                                                     | 29                               |
| 4        | phonotephrite    | 268                   | 12 25 2 186                                                   | 69.4                             |
| 5        | phonolite        | 267                   | 1 236                                                        | 88.4                             |
| 6        | basalt           | 9349                  | 616 271 26 6705 1317 49 365                                   | 71.7                             |
| 7        | trachybasalt     | 1486                  | 259 288                                                      | 44.9                             |
| 8        | basaltic trachyandesite | 1678 | 3 76 1 34 1359 13 4 113 8 67                              | 81.0                             |
| 9        | phonotephrite    | 341                   | 7 94                                                         | 14.4                             |
| 10       | tephriphonolite  | 133                   | 13 6 83                                                      | 62.4                             |
| 11       | basaltic andesite| 3884                  | 2 3 540 254 502 2486 97                                      | 64.0                             |
| 12       | andesite         | 4136                  | 75 258 3653 150                                             | 88.3                             |
| 13       | trachyandesite   | 1538                  | 4 152 25 30 1 173 1142 5 6 74.3                              |
| 14       | trachyte         | 1301                  | 224 18 38 106 65 725 23 102 55.7                           |
| 15       | dacite           | 2750                  | 1134 8 1289 311                                             | 46.9                             |
| 16       | trachydacite     | 224                   | 8 1 42 3 170 75.9                                           |
| 17       | rhyolite         | 3725                  | 93 117 286 3229                                            | 86.7                             |
From the IgRoClaMSys_ilr scheme, 10 subalkali basalt and 1 basaltic andesite samples were classified as such, which represented only about 46% agreement between the two schemes. However, the two schemes provided different names for more (13) samples (Table S76), which once again suggests that the new scheme should be used for the nomenclature of altered rocks.

The final application to Archean mafic magmatism in the Kalgoorlie area of the Yilgarn craton, Western Australia (Application study A5; Fig. 2; Table S77; Bateman et al., 2001). The IUGS scheme indicated that the magma types of 70 samples were distributed as follows: 2 ultrabasic, 31 basic, and 37 intermediate. The IgRoClaMSys_ilr scheme, on the other hand, classified them as 1 ultrabasic, 63 basic, and 6 intermediate rocks (Table S77). Only 30 basic and 5 intermediate rocks were consistently classified by both schemes (IUGS and IgRoClaMSys_ilr). The remaining 35 samples (amounting to 50%) were classified differently (Table S77) for magma types. The two classification schemes differed even more for rock types because 41 samples out of 70 (amounting to 59%) were classified differently (Table S77).

Because the good functioning of the new classification scheme was documented from the initial database as well as 4 independent tests, these significantly higher differences between the new and IUGS schemes for older rocks make it clear that the new scheme (IgRoClaMSys_ilr) should be used for the nomenclature of altered rocks.

We may also mention that the new classification scheme will be useful for hydrothermally or low-grade metamorphic or metasomatic rocks as suggested from their robustness against post-emplacement chemical changes (see the Section of “Robustness of the new multidimensional classification scheme” below). Therefore, the new procedure will be applicable in geothermal or mineral industries for the nomenclature of hydrothermally or metamorphosed or metasomatic igneous rocks.

**Application to Igneous Provenance of Siliciclastic Sediments**

As an innovation, the new IgRoClaMSys_ilr scheme can be used for deciphering igneous provenance of sediments and sedimentary rocks. We illustrate this application from 3 studies (sediment application SA1 to SA3; data from Pinto et al., 2004; Odoma et al., 2015; and Ishiga et al., 2000, respectively). These applications contrast the provenance suggested by the original authors (Pinto et al., 2004; Odoma et al., 2015).

Pinto et al. (2004) presented sediment data from Bolivia and Chile (Fig. 2; adjusted major element chemical data in Table S78). Twelve samples from Bolivia indicated an acid and mainly rhyolitic provenance (12 acid rocks; 8 rhyolites, 3 trachydacite, and 1 dacite; Table S78). On the other hand, 26 Chilean samples were more consistent with an intermediate and andesitic provenance (21 intermediate and 5 acid rocks; 19 andesite, 3 dacite, 1 each basaltic andesite, trachyandesite, trachydacite and rhyolite; Table S78).

The second sediment application study (SA2; Fig. 2; Table S79) concerns sediments from Enugu, southeastern Nigeria (Sediment application study SA2; Odoma et al., 2015). The provenance is likely of basic rocks (6 out of 7 samples; Table S79). More specifically, it appears to be basaltic trachyandesite, mugearite (4 samples; 2 phonolite, and 1 rhyolite; Table S79), i.e., basic alkaline provenance.

The final application is for coastal lagoon sediments from southwest Japan (SA3; Fig. 2; Table S80; Ishiga et al., 2000). The sediment provenance can be inferred as from intermediate rocks (43 out of 49 rocks; about 88%) and more specifically, basaltic andesite rocks (37 out of 49 rocks; about 76%).

Thus, igneous provenance of sediments can be successfully inferred from the IgRoClaMSys_ilr.

**Robustness of the New Multidimensional Classification Scheme**

The additional modules programmed in IgRoClaMSys_ilr enable the user to determine the robustness of their own samples (one at a time) with respect to analytical errors or uncertainties as well as post-emplacement compositional changes such as weathering, hydrothermal alteration or low-grade metamorphic or metasomatic changes. The appropriate templates are included for an efficient use of these capabilities. The user is free to input data of an actual sample in the appropriate Excel file and watch the robustness of the multidimensional procedure.

**Conclusions**

The new multidimensional classification scheme proposed from linear discriminant and canonical analysis of 9 isometric log-transformed ratios of all major elements showed high percent success values (generally > 50%) for most of the 17 root names and 10 sub-root names. New computer program IgRoClaMSys_ilr for online processing of data would facilitate its use by all those interested in correctly classifying old or altered igneous rocks as compared to the IUGS and other alternative procedures. This new scheme would be useful for the classification of weathered, hydrothermally altered or low-grade metamorphic or metasomatic rocks in geothermal or mineral industries.

The available IUGS scheme is certainly suitable for the classification of fresh rocks and was used as a reference for the evaluation of the new scheme. Independent evaluation of the IgRoClaMSys_ilr scheme from data not used for proposing it fully confirmed its good functioning. The application studies documented in this work clearly suggest that the new scheme should be used for the nomenclature of altered igneous rocks. An innovative application was also suggested for inferring igneous provenance of siliciclastic sediments and sedimentary rocks.

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