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Computer programs for the classification and nomenclature of igneous rocks

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We review the most important computer programs for the classification of igneous rocks and point out those that follow the recommendations of the International Union of Geological Sciences (IUGS). A new program "Igneous Rock Classification System" (IgRoCS), written in Visual Basic, is then described in detail. IgRoCS allows the user to follow strictly the IUGS classification and nomenclature scheme for igneous rocks. The special rocks are first classified, then plutonic rocks are named after the IUGS mineralogical classification, next high-Mg and picritic volcanic rocks are identified from the IUGS criteria, and finally other volcanic rocks are classified according to the TAS diagram and CIPW norm. The chemical classification of volcanic rocks can also be achieved directly without going through the classification of other rock types. The IgRoCS program incorporates the revised standard igneous norm. Thus, the use of this new software is encouraged for a strict application of the IUGS recommendations for igneous rock classification and nomenclature.

Introduction

For several decades, the International Union of Geological Sciences (IUGS) has been concerned with an appropriate classification scheme for igneous rocks. Under the umbrella of the IUGS, numerous renowned scientists, such as Albert Streckeisen, Bruno Zanettin, Mike Le Bas, Bernard Bonin, and Roger Le Maitre, among others, have pursued the goal of putting forth a standard procedure for igneous rock classification, which should be followed by everyone.

Thus, on the recommendation of Professor T.F.W. Barth, the Sub-commission on the Systematics of Igneous Rocks was constituted under the IUGS Commission on Petrology, which commenced its work back in 1970.

The Sub-commission commenced with the plutonic rocks and gave its final recommendations as a monumental paper by Streckeisen (1976), which has been highly used, with around 1030 citations in SCI-indexed international journals, as confirmed by us on September 1st, 2012 in the Science Citation Index (SCI) database of the Institute for Scientific Information (ISI), Philadelphia. The large number of

citations in different international journals gives a clear-cut idea of the worldwide use of such work.

The attention of the Sub-commission then shifted to volcanic rocks. Among the several short documents, the most noticeable has been the highly cited publication by Le Bas et al. (1986) specifically geared for the classification of volcanic rocks (with over 1800 citations in international journals SCI-ISI, as on September 1st, 2012). The well-known TAS (Total Alkalis versus Silica) classification, although improperly used by most scientists even today, was the most important outcome of this joint effort. The classification scheme for the high-Mg and picritic volcanic rocks prior to the TAS classification was also put forth by Le Bas (2000), with around 160 citations in international journals.

Similarly, the classification of pyroclastic, charnockitic, carbonatitic, alkaline and other rocks was also considered, and the Sub-commission realized it to be of utmost importance to present the results of classification and nomenclature as a book whose first edition was by Le Maitre et al. (1989), which has been a highly used and cited document (with around 1500 citations). Then appeared the second edition of this book (Le Maitre et al., 2002), with around 460 citations.

In spite of so many citations of the IUGS proposals and recommendations, it appears that the rock classification as practiced by most scientists lacks the rigor suggested by the IUGS proponents. For example, for volcanic rock classification the TAS scheme practiced by most people does not take into account the Fe-oxidation and 100% anhydrous basis adjustments, because the measured SiO₂ and Na₂O+K₂O values are simply plotted, without any thoughts on the interdependency of compositional data and closure problems (Chayes, 1960; Aitchison, 1986; Verma, 2010). It is well known that the sum of the measured major elements (or oxides) is seldom 100% and volatile components may constitute a significant part of this total. Besides, more importantly, both oxidation states (Fe₂O₃ and FeO) are seldom separately measured. Therefore, by the use of measured crude compositions of SiO₂ and Na₂O+K₂O, the recommendations of Le Bas et al. (1986) or Le Maitre et al. (1989, 2002) are not really taken into account in the TAS diagram. Similarly, not all CIPW norm schemes lead to the same answer (Middlemost, 1989; Le Maitre, 2002; Verma et al., 2003). These considerations, therefore, should be a major issue to be addressed, if we were to count on a common "language" for the nomenclature of volcanic rocks.

Existing computer programs

We will concentrate on the characteristics of the existing software

for igneous rock classification and nomenclature, but will not comment on other applications, such as several kinds of simple bivariate, ternary, multi-element normalized, or discrimination diagrams popular among the Earth scientists. The readers can explore these aspects themselves in the computer programs cited in this review, or elsewhere, e.g. Rollinson (1993, a popular book with around 1180 citations in SCI-ISI journals).

WINROCK (1997-2012)

This computer program, initially proposed in 1997, was updated extensively in 2012 (R.A. Kanen; <http://www.geologynet.com>). WINROCK is commercially available as a single user version for AU \$399.00 (<http://www.geologynet.com/order.htm>). It is capable of providing a wide range of IUGS diagrams for rock classification. However, WINROCK does not classify all special rocks suggested by Le Maitre et al. (2002). The program does not validate data for the QAPF diagram. Similarly, for volcanic rock classification the program requires the user to input the Fe-oxidation ratio, because the program does not include the calculation scheme proposed by Le Maitre (1976a) or Middlemost (1989).

Because the program was not published in an international journal, it is not easy to check the impact of this software in terms of total citations in international journals.

IUGSTAS software package (2002)

In Appendix C of the book by Le Maitre et al. (2002), Le Maitre (2002) described a collection of C++ programs (IUGSTAS software package) for implementing the TAS classification for volcanic rocks (Le Bas et al., 1986). According to Le Maitre (2002), this software corrected the then prevailing common mistakes and rounding errors in the CIPW norm (Cross et al., 1902) calculation schemes (Johannsen, 1931; Kelsey, 1965).

This program is available from the Cambridge University Press, as a part of the book by Le Maitre et al. (2002). Although the author stated that he extensively used this code in the CLAIR data system (Le Maitre, 1973, 1976b), its use by others has been rather limited, with the unfortunate consequence that the problem of the incorrect use of the TAS classification still persists.

SINCLAS (2002)

This computer program “Standard Igneous Norm and Volcanic Rock **CL**assification System” (SINCLAS; Verma et al., 2002, 2003), written in Visual Basic, was meant for the classification of volcanic rocks fully consistent with the IUGS recommendations (Le Bas et al., 1986), including the special high-Mg and picritic rocks (Le Bas, 2000), such as meimechite, komatiite, picrite, and boninite. SINCLAS corrects the measured concentrations to 100% on an anhydrous basis after proper Fe-oxidation adjustment (Le Maitre, 1976a; Middlemost, 1989). It also allows the use of actually measured Fe_2O_3 and FeO concentrations. Because Le Bas et al. (1986) also proposed the use of normative minerals for volcanic rock subroot names, SINCLAS allows precise and accurate norm calculations according to the standard igneous norm (a revised CIPW norm) scheme proposed by Verma et al. (2003). Furthermore, this program provides information on the magma type (ultrabasic, basic, intermediate, or acid) from the adjusted compositions. This information has been used for multi-dimensional

tectonomagmatic discrimination diagrams recently proposed for igneous rocks (e.g., Verma, 2010, 2012; Verma and Agrawal, 2011; Verma et al., 2012).

SINCLAS (Verma et al., 2002) is freely available on request to the first author. It has been used in the literature for the TAS diagram and volcanic rock nomenclature (with around 80 citations in SCI-ISI international journals for rock classification purposes). A few years ago, Pruseth (2009) proposed new formulae for the calculation of the CIPW norm and claimed that they performed better than the SINCLAS computer program.

IgPet (2006-2007)

First introduced by Carr (1995), its current updated (2006-2007) version can be purchased as a single user version for US \$199.00 from RockWare Inc., Golden, CO 80401, USA (<http://www.rockware.com>). This program facilitates the TAS classification and CIPW norm calculations, as well as allows the use of some mineralogical diagrams, although the latter do not seem to be those required by the IUGS classification scheme for plutonic rocks. Further, it is not clear if IgPet allows different types of Fe-oxidation adjustments as readily available in SINCLAS.

GCDKit (2003-2011)

GeoChemical Data ToolKit (GCDKit; <http://www.gcdkit.org>), written in language R and first reported by Janousek et al. (2006), has its updated version 3.0 available in 2011 (Janousek et al., 2011). This freely available program is capable of providing the QAPF classification for plutonic (Streckeisen, 1974) and volcanic (Streckeisen, 1978) rocks, TAS diagram (Le Bas et al., 1986; Middlemost, 1994), and the CIPW norm calculations. Other IUGS recommendations such as those for the classification of special rocks are not considered. GCDKit in its first documentation in an international journal (Janousek et al., 2006) did not mention the prior existence of the SINCLAS computer program. Nevertheless, mainly for the purpose of other tasks and not for rock classification, GCDKit has been cited in more than 70 papers in SCI-ISI journals.

PetroGraph (2005)

This freely available software permits rock classification from the TAS diagram, both for volcanic (Le Bas et al., 1986) and plutonic (Cox et al., 1979) rocks. The IUGS recommendations for plutonic rock nomenclature, such as the use of the QAPF double-triangle, cannot be followed. Further, it is not clear if the program allows for the prior adjustment of measured compositions on an anhydrous basis, nor is there any mention of Fe-oxidation ratio adjustment. The authors failed to acknowledge the prior computer program SINCLAS for this purpose. Although not specifically used for rock classification, this program has been cited in around 20 papers included in SCI-ISI journals.

New computer program IgRoCS (2012)

IgRoCS (**I**gneous **R**ock **C**lassification **S**ystem; this work), written in Visual Basic and Net Framework, strictly follows all IUGS recommendations for the classification and nomenclature of igneous rocks (Le Maitre et al., 2002). Figure 1 provides a schematic flow

classification, we compiled in the DataChem_IUGS.xls file geochemical data for 467 representative samples of mostly volcanic rocks. Some intrusive rocks were also included to highlight the use of IgRoCS when the mineralogical information is not available or when the user is interested in deciphering the magma equivalent for their rock samples, particularly for their use in appropriate tectono-magmatic discrimination diagrams (e.g. Verma et al., 2006, 2012; Verma and Agrawal, 2011). Similarly, some older rocks were also included, because no reliable proposal for their classification is yet available (see Verma et al., 2010, for the poor performance of such classification diagrams). Therefore, the TAS and CIPW norm classification can be tentatively used until new multi-dimensional diagrams currently under preparation by S.P. Verma and collaborators are proposed.

For establishing the DataChem_IUGS.xls file, numerous sources were considered to achieve a worldwide representation of all rock types, but at the same time, limiting the total number of samples so that in a TAS diagram the data could be easily visualized. Their sources were as follows (listed alphabetically for the authors): Abdel-Rahman and Lease (2011); Agostini (2003); Agostini et al. (2006, 2007, 2010); Aguirre-Díaz and McDowell (2000); Agustín-Flores et al. (2011); Ahmad et al. (2008); Ahmadian et al. (2009); Akal (2003); Alam et al. (2004); Albrecht and Goldstein (2000); Aldanmaz et al. (2000, 2006, 2008); Alici et al. (2002); Arce et al. (2008); Arnórsson et al. (2002); Arpa et al. (2008); Avanzinelli et al. (2008); Avellán et al. (2012); Ayabe et al. (2012); Ayalew et al. (2006); Aydar et al. (2003); Aydin et al. (2008); Bachmann et al. (2002); Bagci et al. (2008); Bailey et al. (2009); Ban et al. (2007); Barker et al. (2009); Barling et al. (1994); Barrat et al. (2003); Bayat and Torabi (2011); Beccaluva et al. (2002); Beier et al. (2006, 2008); Benoit et al. (2002); Bergmanise et al. (2000); Blatter and Hammersley (2010); Blatter et al. (2001, 2007); Boari et al. (2009); Bolge et al. (2006); Booden et al. (2011, 2012); Bruni et al. (2008); Bryan (2006); Bryant et al. (2006); Cadoux and Pinti (2010); Calmus et al. (2003, 2010);

Carmichael et al. (2006); Carn and Pyle (2001); Carrasco-Núñez et al. (2010); Chadwick et al. (2007); Chakrabarti et al. (2009); Chang et al. (2009); Chen et al. (2012); Churikova et al. (2001); Conly et al. (2005); Conticelli et al. (2009); Coogan et al. (2001); Corgne et al. (2001); Cousens et al. (2003); Çubukçu et al. (2012); Cucciniello et al. (2011); Cunningham et al. (2009); de Lima et al. (2011); Deering et al. (2011, 2012); Dilek et al. (2010); Ding et al. (2003); Dini et al. (2002); Doucelance et al. (2003); Elburg et al. (2003); Elitok et al. (2010); Ferlito et al. (2009); Fontijn et al. (2010); Fretzdorf and Haase (2002); Frey et al. (2000); Gao et al. (2010); García Tovar (2009); Geldmacher and Hoernle (2000); Gorrington and Kay (2001); Guzman et al. (2011); Haase et al. (2002, 2004); Hanyu et al. (2011); Harper (2003); Hawkins and Ishizuka (2009); Hekinian et al. (2003); Hoke and Lamb (2007); Holm et al. (2006); Horz et al. (2004); Hou et al. (2004); Hsu et al. (2000); Ilbeyli et al. (2004); Ireland et al. (2009); Ishizuka et al. (2002); Jian et al. (2009); Jorgensen and Holm (2002); Jutzeler et al. (2010); Karsli et al. (2008); Kawabata et al. (2011); Kerrich and Manikyamba (2012); Kim et al. (2008); Kimura et al. (2001); Koprubasi and Aldanmaz (2004); Krochert and Buchner (2009); Ma et al. (2011); Mahéo et al. (2009); Manikyamba et al. (2005); Marshall et al. (2009); Martynov et al. (2010); Massaferrero et al. (2006); Melluso et al. (2010); Nikogosian and Van Bergen (2010); Nonnotte et al. (2011); Ortiz-Hernández et al. (2003); Owen (2008); Özdemir et al. (2011); Pappalardo et al. (2008); Patino et al. (2003); Peccerillo et al. (2003); Perini et al. (2004); Polat et al. (2002); Price et al. (2003); Ren et al. (2004); Robin et al. (2009); Rogers et al. (2004); Rolland et al. (2009); Rollinson (2009); Ronga et al. (2010); Rooney et al. (2007); Rosa et al. (2004, 2006); Schaaf et al. (2005); Schuth et al. (2004, 2009); Shane et al. (2005); Sheth and Melluso (2008); Sheth et al. (2003); Shinjo et al. (2011); Shukuno et al. (2006); Siebert and Carrasco (2002); Spath et al. (2001); Srivastava (2006); Sruoga et al. (2005); Tamura et al. (2009); Tatar et al. (2007); Taylor et al. (1994); Tian et al. (2011); Torabi (2009); Turner et al. (2012); Upton et al. (2000); Verma (2000); Vigouroux et al. (2008); Wang et

Figure 2. The TAS diagram for the samples compiled in DataChem_IUGS.xls file. See text for the literature source of data. Filled black circles show the high-Mg and picritic rocks, whereas symbols used for other rock types are self-explanatory. The abbreviations used are the same as in Verma et al. (2002): A = Andesite, B = Basalt, BA = Basaltic andesite, BSN = Basanite, BTA = Basaltic trachyandesite, D = Dacite, FOI = Foidite, PB = Picrobasalt, PH = Phonolite, PHT = Phonotephrite, R = Rhyolite, T = Trachyte, TA = Trachyandesite, TB = Trachybasalt, TD = Trachydacite, TEP = Tephrite, and TPH = Tephriphonolite.

al. (2012); Watts et al. (2011); Zaitsev et al. (2012); Zellmer and Turner(2007); Zellmer et al. (2000); Zhang et al. (2003); Zongfeng et al. (2009); and Zou et al. (2003, 2008).

IgRoCS automatically classified all samples and assigned appropriate IUGS rock names to them. The resulting TAS diagram is presented in Fig. 2. The choice of samples confirmed that all rock types were represented in this example file (DataChem_IUGS.xls).

IgRoCS can automatically process any number of samples in a single run, which is an advantage over SINCLAS when one is interested in processing large databases. IgRoCS, therefore, provides an unparallel advantage for the IUGS igneous rock classification as compared to all existing computer programs. IgRoCS is available on request to any of the authors.

Conclusions

Several computer programs, viz., WINROCK, IUGSTAS, SINCLAS, IgPet, GCDKit, PetroGraph, and IgRoCS, are available specifically for the IUGS classification and nomenclature of igneous rocks, of which IgRoCS presented in this paper seems to be the most versatile and useful program for strictly following the IUGS recommendations. WINROCK and IgPet are commercial software, whereas IUGSTAS, SINCLAS, GCDKit, PetroGraph, and IgRoCS are freely available.

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