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Development of System and Software

A NEW SOFTWARE PACKAGE FOR RITTMANN NORM CALCULATION

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Abstract : MRittmann is a petrological software package for identifying and calculating the normative minerals of volcanic, sub-plutonic, and carbonatite rocks from bulks chemical analyzes. The calibration of the software is built on the Rittmann norm calculation principles, and its calculating results include both hydrous and anhydrous minerals, rock name as well as petrological index such as tau (τ) and degree of oxidation (Ox^0) of the analyzed samples. The norms obtained from MRittmann are in volume percentages. They are close to the modes and convenience for petrologist to use in graphical purposes in term of plotting the analyzed rock in QAPF double-triangle. The program is written in Delphi for PC and compatibles, and runs under Windows 9x, 2000, NT operating systems. The first version of MRittmann, MRittmann 1.0® was released by Duong The Hung and Dam Quang Minh at the Faculty of Geology, Hanoi University of Science, with all copyrights reserved.

Key words : Igneous petrology, Bulks chemical analysis, Rittmann norms, QAPF double-triangle

1. INTRODUCTION

To handle the igneous crystallization process through the petro-chemistry aspect, a procedure was developed to reduce all igneous rocks to a basis that depends on chemistry only. This procedure is for converting the chemical composition of an igneous rock to an ideal mineral composition, a mineralogical norm. The CIPW norms, named after Whitman Cross, Joseph P. Iddings, Louis V. Pirsson, and Henry S. Washington who devised the procedure, was used over eighty years ago.

This CIPW norm based on a number of simplifications: (1) the magma crystallizes under anhydrous conditions and at low pressure, consequently no hydrous minerals such as hornblende, biotite are formed; (2) the ferromagnesian minerals are assumed to be free of Al_2O_3; (3) for all ferromagnesian minerals, the Fe/Mg ratio is set to be the same; and (4) several minerals pairs are assumed to be mutually exclusive, for example, nepheline or olivine never appear with quartz in the norm.

Being developed in 1973 by Rittmann (1973), the Rittmann norm has come over above simplifications, and has been devised for high-pressure or very hydrous situations. But the norm would be extremely complex to calculate, and calculating it is a quite time-consuming work. Therefore, the MRittmann 1.0 computer program was built to calculate the norm of volcanic and sub plutonic rocks based on the Rittmann's method.

2. PRINCIPLES AND GENERAL CALCULATION PROCEDURE

MRittmann 1.0 was programmed on the principles of Rittmann norm calculation. Details of the norm calculation had been published on Rittmann (1973). In this paper, the principles will be briefly restated from the work with some additional comparison to those of CIPW norm.

The mineralogy of an igneous rock is a complex function of its chemistry and crystallization history. In the purpose of being close to what really happened in the nature of crystallizing process, MRittmann based on the five principles as follows:

In contrast to the CIPW norm, which is based on simple stoichiometric compounds, Rittmann norm calculation is essentially empirical in character and uses average compositions of the actual minerals.

Unit of calculation is not the chemical formula of a mineral but the single electropositive contained in the mineral (CO_3^{2-} and SO_4^{2-} also be counted). For example, $KAlSi_3O_8$ = 5 Or ; or with the average composition of natural leucite, the reaction between leucite and quartz to form K-feldspar will be expressed as:

$$K_{10}NaAl_{11}Si_{22}O_{66} + 11\ SiO_2 = K_{10}NaAl_{11}Si_{33}O_{88} \quad \cdots\cdots\cdots (1)$$

$$11\ Lc + 11\ Q = 55\ \text{Sanidine (San)} \quad \cdots\cdots\cdots (2)$$

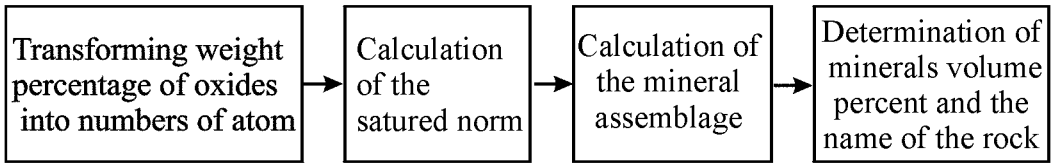

Figure 1. Norm calculation procedure of MRittmann 1.0.

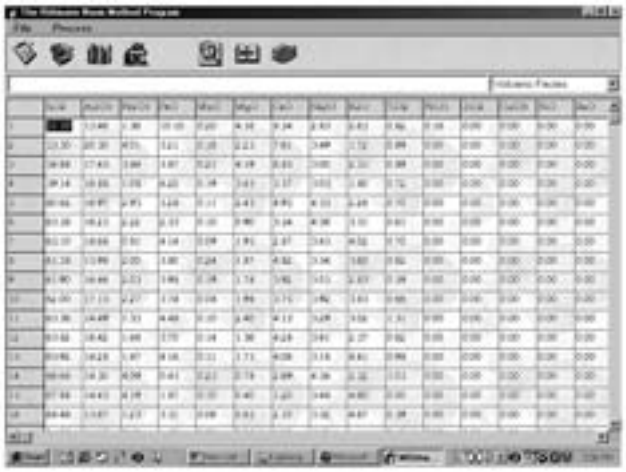

Figure 2. Input screen of MRittmann 1.0.

Figure 3. Output screen of MRittmann 1.0.

Number of atoms = weight percentage of an oxide divided by molecular weights per number of electropositive. While in the CIPW norm, not the number of atom but the molar oxide proportions will be calculated by taking the oxide weight percents in the chemical analysis and divide them by their respective formula weights.

Degree of oxidation $Ox^0 = Fe^{3+} / (Fe^{3+} + Fe^{2+} + Mn)$ will be one of the important index in the norm calculation. This index characterizes for magma differentiations. It controls the formation of magnetite and is the determination factor for secondary alteration.

Saturated norm: "the Saturated norm serves as a basis for the calculation of the stable mineral assemblages for all facies of igneous rocks" (Rittmann, 1973). It is calculated "by distributing the number of atoms among saturated silicates, accessory minerals and occasional compounds, without considering the available amount of Si" (Rittmann, 1973). The norm calculation procedure is shown in Figure 1.

3. THE COMPUTER PROGRAM

MRittmann 1.0 was built in order to electronically process the complicated calibration of the Rittmann norm calculation. It was programmed in Delphi programming language, with the size of 2.7 MB, and run in the Microsoft Window environment.

Input data (Figure 2):

- Weight percentages of twelve major element oxides;
- Type of rock forming condition: volcanic, "wet" subvolcanic facies, "dry" subvolcanic facies, or carbonatite

The input data file is read from the keyboard or from an existing data file on the disk. More than thousand of analyzed samples can be stored in a file.

Output data (Figure 3):

- The norm in volume percentages and the rock name as the result of the program are outputted in one page per analysis on screen or printer.
- At the end of the outputted page, three index of the rock sample also be added to the result, namely sigma (σ): serial index: $(Na_2 + K_2O)/ (SiO_2 - 43)$; tau ($\tau$):$(Al_2O_3 - Na_2O)/ TiO_2$; and degree of oxidation: Ox^0

Examples of input and output screen are shown on the Figure 2 and Figure 3.

Even though we consider that the present program MRittmann presented in this paper is reliable, we compare its calculation results (Table 3) with that by the author of the Rittmann method (Table 2) and by other norm-calculation computer programs (Table 4, Table 5).

Bulk chemical compositions of six different rocks have been inputted for the MRittmann 1.0 and three other software which used the CIPW norm: Norm3 (Kurt Hollocher, 1999); Chempet (Yegorov *et al*., 1996) and Norma (Hualde, 1994). The first three bulk chemical compositions are of the rocks that Rittmann (1973) had used for his calculation 30 years ago (Table 1), and the other ones (Table 6) are of the rocks, that were so called lamproite, in the west northern part of Vietnam.

The results have shown some valuable similarities as well as differences. These calculations clearly indicate that the results by the MRittmann program conforms to Rittmann and other CIPW-based programs.

Table 1. Chemical bulk analyses of the 3 selected rocks (Rittmann , 1973) .

No	SiO_2	TiO_2	Al_2O_3	Fe_2O_3	FeO	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	H_2O
1	74.93	0.13	13.52	0.76	0.72	0.08	0.32	0.93	4.50	3.39	0.08	0.79
2	50.52	1.24	17.67	4.57	6.98	0.18	5.06	8.98	2.80	0.58	0.23	1.17
3	48.67	2.28	15.91	3.24	7.13	0.15	7.72	8.02	4.26	1.28	0.62	1.06

Table 2. Rittmann norm of the 3 selected rocks in table 1, calculated by Rittmann (1973).

No	Qtz	Sa	Pl	Nph	Hau	Cpx	Ol	Bt	Crd	Mnh	Ill	Apt	Ant	CI	σ	τ
1	32.7	42.6	19.9	0	0	0	0	2.1	2.3	0.2	0	0.2	11	4.8	1.9	69.4
2	4.1	0	67	0	0	24.1	0	0	0	2.9	1.3	0.5	54	28.9	1.5	12
3	0	5.1	60.4	2.5	0	13.7	12.3	0	0	2.5	2.2	1.3	34	32	5.4	5.1

Table 3a. Norm of the three selected rocks in table 1, calculated by MRittmann 1.0.

No	Qtz	Orth	Ab	Ant	Bt	Zr	Apt	Ilm	Mnh	Sil	Crd	Hyp	Cpx	Nph	Ol	Oxi	Tau	Delta
1	32.6	19.4	38.6	3.9	2.1	0.7	0.2	0.1	0.2	0.0	2.4	0.0	0.0	0.0	0.0	32.6	19.4	38.6
2	1.3	3.9	27.1	36.2	0.0	1.2	0.5	1.4	1.6	0.0	0.0	18.9	8.0	0.0	0.0	1.3	3.9	27.1
3	0.0	8.2	33.7	20.7	0.0	1.1	1.3	2.2	1.6	0.0	0.0	0.0	13.5	4.1	0.0	0.0	8.2	33.7

Table 3b. Name of rocks samples in table 3a, determined by MRittmann 1.0.

Sample No	Rock name	Sample No	Rock name	Sample No	Rock name
1	Tephrinephilinite tephrileucite	2	Andesite	3	Latibasalt

Table 4. Norm of the three selected rocks in table 1, calculated by NORMA program.

No	Qtz	Orth	Ab	An	Hyp	Nph	Di	Mnh	Ol	Ilm	Apt	Crn
1	33.3	20.0	38.1	4.1	1.4	0.0	0.0	1.1	0.0	0.3	0.2	1.0
2	4.5	3.4	23.7	33.9	16.3	0.0	7.4	6.6	0.0	2.4	0.5	0.0
3	0.0	7.6	31.4	20.5	0.0	2.5	12.2	4.7	14.6	4.3	1.4	0.0

Table 5. Norm of the three selected rocks in table 1, calculated by CHEMPET program.

No	Qtz	Ab	An	En	Fs	Hyp	Hd	Fo	Fa	Ilm	Mnh	Di	As
1	43.4	38.1	4.6	0.8	0.6	1.4	0.0	0.0	0.0	0.3	1.1	0.0	7.0
2	6.1	23.7	35.7	10.4	6.0	16.4	2.4	0.0	0.0	2.4	6.6	4.8	0.0
3	0.0	38.1	23.0	6.3	2.9	9.2	3.8	0.7	0.4	6.3	6.0	9.7	0.0

Table 6. Chemical bulk analyses of the rocks, so called Lamproite, in the West Northern part of Vietnam (Thuyet, 2001).

No	SiO_2	TiO_2	Al_2O_3	Fe_2O_3	FeO	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	h.k.l
K2199	50.62	0.5	10.4	7.3	-	0.1	11.3	7.8	2.1	6.4	0.5	1.4
P178	52.12	0.7	12.4	7.6	-	0.2	9.27	7.6	0.9	5.5	0.5	2.9
H573	53.48	0.6	11.4	7.8	-	0.1	10.7	7.3	2.2	5.1	0.4	0.8

Table 7. Norm of the rocks in table 6, calculated by MRittmann 1.0.

No	Orth	Ab	Anth	Ol	Cpx	Hyp	Leu	Apt	Mnh	Ilm	Rock name	Oxi	Tau	Delta
K2199	16.4	14.6	0.0	13.7	30.0	0.0	22.8	1.1	2.0	0.0	Tephriphonolite	1.0	16.6	0.5
P178	37.6	8.7	13.5	1.8	19.9	17.0	0.0	1.1	1.6	0.9	Tephriphonolite	1.0	12.8	0.1
H573	33.8	20.0	5.2	11.3	23.0	3.7	0.0	0.9	1.9	0.3	Tephriphonolite	1.0	15.3	0.5

Table 8. Mineral's abbreviation used in the paper.

Minerals	Ab.	Minerals	Ab.	Minerals	Ab.	Minerals	Ab.	Minerals	Ab.	Minerals	Ab.
Albite	Ab	Alumosilicates	As	Diopside	Di	Hauyne	Hau	Magnetite	Mnh	Quartz	Qtz
Albite	Ab	Biotite	Bt	Enstatite	En	Hedenbergite	Hd	Nepheline	Nph	Sanidine	Sa
Anortite	An	Clinopyroxene	Cpx	Fayalite	Fa	Hyperthen	Hyp	Olivine	Ol	Sillimanite	Sil
Anorthoclase	Anth	Cordierite	Crd	Forsterite	Fo	Ilmenite	Ilm	Orthoclase	Orth	Zircon	Zr
Apatite	Apt	Corundum	Crn	Ferrosilite	Fs	Leucite	Leu	Plagioclase	Pl		

From the above results of calculation, it can be noted that there are some petrological distinguished features of the norms calculated by MRittmann program.

Firstly, in the MRittmann procedure, the final tally of normative minerals is expressed in volume units (volume percentage). It is considered very helpful to know the volume proportions of the normative minerals for comparison with rock modes.

In addition, norms from MRittmann are expressed in terms of both anhydrous and hydrous minerals. It is the fact that many igneous rocks in the nature are composed of micas or amphiboles that do contain water inside. These minerals are used in the Rittmann norms but not the CIPW ones. In a rock, which is peraluminous ($Al_2O_3 > K_2O + Na_2O + CaO$), there will be corundum and no wollastonite, no diopside in the norm. The norm of a peralkaline rock ($Al_2O_3 < K_2O + Na_2O$) will contain acmite and no anorthite. In a wet rock, muscovite will appear instead of corundum and biotite instead of hypersthene, particularly with a wet peralkaline rock, amphibole in term of arfvedsonite or riebeckite would coexist with aegirine-augite and alkali feldspar, but plagioclase will not be presented.

4. CONCLUSION

MRittmann is very useful software for petrological studies. It produces results that match with the observed mineral phases perfectly. However, as noted by Gottini (1973), both types of norms are fundamentally different from each other and are based on different principles. They are not antithetical but complementary. For the discussion of purely petrochemical problems, the CIPW norm is very useful, whereas the Rittmann norm serves for petrographical purposes, such as the correct denomination and systematic position of volcanic rocks that mostly do not permit a complete determination of their modes. For more information on the availability contact either of the authors.

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