Calculation of the CIPW norm: New formulas

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A completely new set of formulas, based on matrix algebra, has been suggested for the calculation of the CIPW norm for igneous rocks to achieve highly consistent and accurate norms. The suggested sequence of derivation of the normative minerals greatly deviates from the sequence followed in the classical scheme. The formulas are presented in a form convenient for error-free implementation in computer programs. Accurate formulas along with the use of variable molecular weights for CaO and FeO; corrected formula weights for apatite, pyrite and fluorite; and suggested measures to avoid significant rounding off errors to achieve absolute match between the sum of the input weights of the oxides and the sum of the weights of the estimated normative minerals. Using an analogous procedure for determining the oxidation ratios of igneous rocks as used in the SINCLAS system of Verma *et al* (2002, 2003), the suggested calculation scheme exactly reproduces their results except for apatite for reasons explained in the text, but with a superior match between the totals for about 11,200 analyses representing rocks of a wide range of composition.

1. Introduction

The CIPW norm provides the basis for the comparison of aphanitic igneous rocks with their phaneritic counterparts. However, the main application of it is in the classification of glassy and very fine-grained volcanic rocks where classification from the evaluation of the mode is not possible (see Verma *et al* 2003 for a detailed discussion). Therefore, to achieve consistency in classification, a standard igneous norm calculation method is essential (Middlemost 1989). Now-a-days norms are usually calculated using digital computers. The classic norm calculation procedure (Cross *et al* 1902) and its later modifications (Washington 1917; Johannsen 1931; Hutchison 1974; Cox *et al* 1979; Le Maitre 1982; Ragland 1989; Rollinson 1993) however, are not specifically suitable for implementation on a computer leading to different methods of implementation by different programmers. Kelsey (1965) modified the portions used especially for the estimation of silica undersaturated minerals in the norm. These modifications however, are not universally adopted in the computer programs

that are available for calculation of the norm. The SINCLAS implementation of Verma *et al* (2002, 2003) which is based and modified after Kelsey (1965) is the most reliable and consistent of all.

Additionally, there is no unique way of fixing the FeO/Fe_2O_3 ratios (oxidation ratios) of igneous rocks which in turn, significantly change the nature and amount of the normative minerals of rocks (Middlemost 1989). Therefore no standardization is possible without evolving a universally agreed procedure to determine the oxidation ratio. Oxidation ratios obtained from chemical analysis either are not acceptable as most of the igneous rocks show higher Fe_2O_3 in their analysis because of the oxidation postdating their consolidation. Until a method is evolved to uniquely fix the oxidation ratio, standardization can only be achieved for the details of the calculation procedure. The SINCLAS system of Verma *et al* (2002, 2003) even offers three options on how to fix the FeO/Fe_2O_3 ratios and involves an amount of subjectivity on the part of the user.

At the end of the calculation of norm for a rock it is customary to report the sum of weights of

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Table 1. *Composition and inverse composition matrices for the saturated normative minerals.*

	C	Or	Ab	An	En	Fs	Hm
Al_2O_3	1	1	1	1	0	0	0
Fe_2O_3	0	0	0	0	0	0	1
FeO	0	0	0	0	0	1	0
MgO	0	0	0	0	1	0	0
CaO	0	0	0	1	0	0	0
Na_2O	0	0	1	0	0	0	0
K_2O	0	1	0	0	0	0	0
	Al_2O_3	Fe_2O_3	FeO	MgO	CaO	Na_2O	K_2O
C	1	0	0	0	−1	−1	−1
Or	0	0	0	0	0	0	1
Ab	0	0	0	0	0	1	0
An	0	0	0	0	1	0	0
En	0	0	0	1	0	0	0
Fs	0	0	1	0	0	0	0
Hm	0	1	0	0	0	0	0

the normative minerals and to compare this value with the sum of weights of the oxides obtained from chemical analysis. Le Maitre (1982) lays great emphasis on the necessity of match between the two up to at least the third place of decimal. Very often this practice offers a means of checking the accuracy of the norm calculation, but the mismatch is not always due to the inaccuracy in the values of the estimated norms. However, perfect match between the two totals imparts a sense of confidence to the calculation and a standard norm calculation procedure should be able to exactly account for the disagreement between the two sums.

It is also observed that not all the computer programs available for the calculation of norm, work satisfactorily over the whole range of composition of igneous rocks. This is probably due to the error-prone schemes and complex decision making steps involved in the calculation of the norms.

Here, a completely new set of formulas has been suggested, based on linear algebraic and mass balance approaches, which are easily understandable and will therefore, lead to less error-prone implementation on a computer. Extension of the classic scheme is also suggested to take care of extremely SiO_2-poor rocks in which the deficiency in SiO_2 cannot be completely compensated for even after converting all leucite to kaliophilite. Additionally, further causes of mismatch between the totals of oxides and normative minerals have been discussed, which when taken care of, achieve an absolute match between the two. The norm calculation steps have been presented in a manner so as to provide maximum convenience in implementing

them on a computer and to avoid ambiguity as far as possible.

2. The method

The composition of the saturated normative minerals can be represented by a composition matrix as given in table 1. The inverse composition matrix (table 1) can be multiplied on the left of a column matrix that contains the analysis of Al_2O_3, Fe_2O_3, FeO, MgO, CaO, Na_2O and K_2O in terms of their molecular proportions obtained by dividing the weight percentages by their respective molecular weights. From the inspection of the inverse composition matrix, it is evident that the same can be written in terms of the following formulas to obtain the provisional saturated minerals.

$$Or_p = K_2O, \qquad Ab_p = Na_2O,$$

$$An_p = CaO, \qquad En_p = MgO,$$

$$Fs_p = FeO, \qquad Hm_p = Fe_2O_3,$$

$$C_p = Al_2O_3 - CaO - Na_2O - K_2O$$

The mineral symbols are given in table 2. The subscript p stands for 'provisional', and numerical subscripts whenever used for intermediate values.

If provisional corundum C_p is negative, then some of the provisional minerals are broken down in specific order one by one to produce

Table 2. *List of oxides with their molecular weights (based on IUPAC Commission on Atomic Weights and Isotopic Abundances; Vocke 1999) and normative minerals and their formulas used in the calculation of the norm.*

SiO_2	60.0843	Quartz (q)	SiO_2
TiO_2	79.8658	Corundum (c)	Al_2O_3
Al_2O_3	101.9613	Zircon (z)	$ZrO_2 \cdot SiO_2$
Fe_2O_3	159.6882	Orthoclase (or)	$K_2O \cdot Al_2O_3 \cdot 6SiO_2$
FeO	71.8444	Albite (ab)	$Na_2O \cdot Al_2O_3 \cdot 6SiO_2$
MnO	70.93745	Anorthite (an)	$CaO \cdot Al_2O_3 \cdot 2SiO_2$
NiO	74.6928	Leucite (lc)	$K_2O \cdot Al_2O_3 \cdot 4SiO_2$
MgO	40.3044	Nepheline (ne)	$Na_2O \cdot Al_2O_3 \cdot 2SiO_2$
CaO	56.0774	Kaliophilite (kp)	$K_2O \cdot Al_2O_3 \cdot 2SiO_2$
BaO	153.3264	Acmite (ac)	$Na_2O \cdot Fe_2O_3 \cdot 4SiO_2$
SrO	103.6194	Sodium metasilicate (ns)	$Na_2O \cdot SiO_2$
Na_2O	61.97894	Potassium metasilicate (ks)	$K_2O \cdot SiO_2$
K_2O	94.196	Diopside (di)	$CaO \cdot (Mg, Fe)O \cdot 2SiO_2$
P_2O_5	141.9445	Wollastonite (wo)	$CaO \cdot SiO_2$
S	32.066	Hypersthene (hy)	$(Mg, Fe)O \cdot SiO_2$
Cr_2O_3	151.9904	Olivine (ol)	$2(Mg, Fe)O \cdot SiO_2$
F	18.9984	Dicalcium silicate (cs)	$2CaO \cdot SiO_2$
CO_2	44.0095	Magnetite (mt)	$FeO \cdot Fe_2O_3$
ZrO_2	123.2228	Chromite (cm)	$FeO \cdot Cr_2O_3$
		Ilmenite (il)	$FeO \cdot TiO_2$
		Hematite (hm)	Fe_2O_3
		Titanite (tn)	$CaO \cdot TiO_2 \cdot SiO_2$
		Perovskite (pf)	$CaO \cdot TiO_2$
		Rutile (ru)	TiO_2
		Apatite (ap)	$9CaO \cdot 3P_2O_5 \cdot CaF_2$
		Fluorite (fr)	CaF_2
		Pyrite (py)	FeS_2
		Calcite (cc)	$CaO \cdot CO_2$

Al_2O_3-undersaturated minerals until the deficiency in Al_2O_3 is resolved. For example, anorthite $(CaAl_2Si_2O_8)$ can be partly or fully converted to wollastonite $(CaSiO_3)$. An and Wo can be represented by the equations:

$$An = 0Al_2O_3 + 1CaAl_2Si_2O_8 = 0C_p + 1An_p$$

and

$$Wo = 1CaAl_2Si_2O_8 - 1Al_2O_3 - SiO_2$$
$$= 1An_p - 1C_p - 1Q_p.$$

The composition and inverse composition matrices representing this breakdown reaction can be written as below. Note that SiO_2 and Q are not

represented in the composition matrix as it is intended here to adjust the Al_2O_3 component. The gain in SiO_2 is finally taken into account in the estimate of quartz (Q), after all other silicate phases have been estimated.

	An	Wo
C_p	0	−1
An_p	1	1

	C_p	An_p
An	1	1
Wo	−1	0

The new estimates of An and Wo are calculated according to the inverse matrix as $An = C_p + An_p$

and Wo $= -C_p$. Once the deficiency of Al_2O_3 is fully resolved, the amount of SiO_2 consumed by the provisional minerals is calculated and if it is found greater than the SiO_2 content of the rock whose norm is being calculated, SiO_2-undersaturated phases are calculated sequentially until the deficiency is completely removed. For example, olivine $((Mg, Fe)_2SiO_4)$ is formed by breaking down provisional hypersthene $((Mg, Fe)SiO_3)$ using the formulas, $Ol = -Q$ and $Hy = 2Q + Hy_p$ according to the matrices,

	Ol	Hy
Q	−1	0
Hy_p	2	1

	Q	Hy_p
Ol	−1	0
Hy	2	1

where, Q represents the deficiency of SiO_2. If Hy is found to be negative after this step, further desilication reactions are required, for example,

$$Ol = 0.5Hy_p$$

$$Ne = -0.25Q - 0.125Hy_p$$

$$Ab = 0.25Q + 0.125Hy_p + Ab_p$$

for which the matrices are,

	Ol	Ne	Ab
Q	−1	−4	0
Hy_p	2	0	0
Ab_p	0	1	1

	Q	Hy_p	Ab_p
Ol	0	0.5	0
Ne	−0.25	−0.125	0
Ab	0.25	0.125	1

Likewise, amounts of the other SiO_2-undersaturated phases are determined. Finally, for extremely SiO_2-undersaturated rocks one further step has been added in which anorthite is broken down to dicalcium silicate and corundum according to the composition and inverse composition matrices:

	Cs	C	An
Q	0	−1.5	0
Cs_p	1	−0.5	0
An_p	0	1	1

	Q	Cs_p	An_p
Cs	−1/3	1	0
C	−2/3	0	0
An	2/3	0	1

The addition of this step is justified by the observation of Al_2O_3-enrichment of pyroxenes and breakdown of early formed anorthites in SiO_2-poor rocks (Carmichael *et al* 1970).

Equations used to construct the composition matrices are given in table 3. Also are given the step numbers where the formulas derived from these equations have been used in the following section.

3. Calculation steps

The oxides and their molecular weights employed in the calculation of the norm are given in table 2. The normative minerals considered, and their formulas and symbols are also given. While Kelsey (1965) used $3CaO \cdot P_2O_5 \cdot 1/3CaF$ for apatite, Verma *et al* (2002, 2003) have used $3CaO \cdot P_2O_5 \cdot 1/3CaF_2$ which is the correct formula. Verma *et al* (2002, 2003) also used a formula $3CaO \cdot P_2O_5 \cdot 1/3CaO$ in the absence of analytical data on F which is most often the case. The latter, however, is not necessary and the standard formula should be used instead. In the present study the formula of $9CaO \cdot 3P_2O_5 \cdot CaF_2$ has been used and the discrepancy arising due to the absence of data on F is taken care of in the final sum of the normative minerals. Let us consider a rock of the following composition. The result of calculation at each step is given in a box.

Oxides	Wt.%
SiO_2	28.03
TiO_2	0.97
Al_2O_3	7.84
FeO	57.27
MgO	0.50
CaO	4.27
K_2O	0.45
P_2O_5	0.39
Total	99.72

Table 3. *Equations used to construct the composition matrices and the step numbers at which the formulas derived from their inverse matrices have been used.*

Steps	Equations
Step 3	$An = 0C + 1An$
	$Wo = -1C + 1An$
Step 4	$Wo = -1C + 1An + 0Ab + 0Hm$
	$Ab = 0C + 0An + 1Ab + 0Hm$
	$Hm = 0C + 0An + 0Ab + 1Hm$
	$Ac = -1C + 0An + 1Ab + 1Hm$
Step 6	$Ab = 0C + 1Ab$
	$Ns = -1C + 1Ab$
Step 7	$Ns = -1C + 1Ab + 0Or$
	$Or = 0C + 0Ab + 1Or$
	$Ks = -1C + 0Ab + 1Or$
Steps 11 and 13	$Ol = -1Q + 2Hy$
	$Hy = 0Q + 1Hy$
Step 14	$Ol = -1Q + 2Hy + 0Ab$
	$Ne = -4Q + 0Hy + 1Ab$
	$Ab = 0Q + 0Hy + 1Ab$
Step 15	$Ol = -1Q + 2Hy + 0Ab + 0Or$
	$Ne = -4Q + 0Hy + 1Ab + 0Or$
	$Lc = -2Q + 0Hy + 0Ab + 1Or$
	$Or = 0Q + 0Hy + 0Ab + 1Or$
Step 16	$Ol = -1Q + 2Hy + 0Ab + 0Or + 0Wo$
	$Ne = -4Q + 0Hy + 1Ab + 0Or + 0Wo$
	$Lc = -2Q + 0Hy + 0Ab + 1Or + 0Wo$
	$Cs = -1Q + 0Hy + 0Ab + 0Or + 2Wo$
	$Wo = 0Q + 0Hy + 0Ab + 0Or + 1Wo$
Step 17	$Ol = -1Q + 2Hy + 0Ab + 0Or + 0Di$
	$Ne = -4Q + 0Hy + 1Ab + 0Or + 0Di$
	$Lc = -2Q + 0Hy + 0Ab + 1Or + 0Di$
	$Cs = -1Q - 2Hy + 0Ab + 0Or + 2Di$
	$Di = 0Q + 0Hy + 0Ab + 0Or + 1Di$
Step 18	$Ol = -1Q + 2Hy + 0Ab + 0Or + 0Di$
	$Ne = -4Q + 0Hy + 1Ab + 0Or + 0Di$
	$Lc = -2Q + 0Hy + 0Ab + 1Or + 0Di$
	$Cs = -1Q - 2Hy + 0Ab + 0Or + 2Di$
	$Kp = -4Q + 0Hy + 0Ab + 1Or + 0Di$
Step 20	$Cs = 0Q + 1Cs + 0An$
	$C = -\frac{3}{2}Q - \frac{1}{2}Cs + 1An$
	$An = 0Q + 0Cs + 1An$

1. Convert the weight percents of the oxides to mole numbers by dividing by the respective molecular weights.
   Add moles MnO and NiO to moles FeO. Add moles BaO and SrO to moles CaO.

Oxides	Moles
SiO_2	0.466511
TiO_2	0.012145
Al_2O_3	0.076892
FeO	0.797139
MgO	0.012406
CaO	0.076145
K_2O	0.004777
P_2O_5	0.002748

Calculate the minerals Z, Py, Cm, Ap, Cc and Il as given below and adjust the amounts of SiO_2, FeO and CaO to be used for further calculations.

$$Z_1 = ZrO_2, \qquad SiO_2 = SiO_2 - Z_1,$$

$$Py_1 = \frac{S}{2}, \qquad Cm_1 = Cr_2O_3,$$

$$FeO = FeO - Py_1 - Cm_1, \qquad Ap_1 = \frac{P_2O_5}{3},$$

$$Cc_1 = CO_2, \qquad Fr_1 = \frac{F}{2},$$

$$CaO = CaO - 10Ap_1 - Cc_1 - Fr_1$$

$$Il_1 = TiO_2$$

$Z_1 = 0$, $SiO_2 = 0.466511$

$Py_1 = 0$, $Cm_1 = 0$, $FeO = 0.797139$

$Ap_1 = 0.000916$, $Cc_1 = 0$, $Fr_1 = 0$,

$CaO = 0.066985$

$Il_1 = 0.012145$
---

2. Calculate the provisional SiO_2 and Al_2O_3 saturated minerals as follows:

$$Or_p = K_2O, \quad Ab_p = Na_2O, \quad An_p = CaO,$$

$$En_p = MgO, \quad Fs_p = FeO, \quad Hm_p = Fe_2O_3,$$

$$C_p = Al_2O_3 - CaO - Na_2O - K_2O$$

$Or_p = 0.004777$, $Ab_p = 0$, $An_p = 0.066986$

$En_p = 0.012406$, $Fs_p = 0.797139$, $Hm_p = 0$

$C_p = 0.005128$
---

3. If $C_p < 0$:

$$An_1 = C_p + An_p \quad \text{else} \quad An_1 = An_p$$

$$Wo_1 = -C_p \quad \text{else} \quad Wo_1 = 0$$

$$\boxed{\begin{aligned} An_1 &= 0.066986 \\ Wo_1 &= 0 \end{aligned}}$$

4. If $An_1 < 0$:

$$Wo_2 = An_p \quad \text{else} \quad Wo_2 = Wo_1$$

$$Ab_1 = C_p + An_p + Ab_p \quad \text{else} \quad Ab_1 = Ab_p$$

$$Hm_1 = C_p + An_p + Hm_p \quad \text{else} \quad Hm_1 = Hm_p$$

$$Ac_1 = -C_p - An_p \quad \text{else} \quad Ac_1 = 0$$

$$\boxed{\begin{aligned} Wo_2 &= 0 \\ Ab_1 &= 0 \\ Hm_1 &= 0 \\ Ac_1 &= 0 \end{aligned}}$$

5. If $Hm_1 < 0$:

$$Ac_2 = Hm_p \quad \text{else} \quad Ac_2 = Ac_1$$

$$Hm_2 = Hm_p - Ac_2$$

$$Ab_2 = Ab_p - Ac_2$$

$$\text{if } An_1 < 0, \quad C_1 = An_1 + Ac_2 \quad \text{else} \quad C_1 = 0$$

$$\boxed{\begin{aligned} Ac_2 &= 0 \\ Hm_2 &= 0 \\ Ab_2 &= 0 \\ C_1 &= 0 \end{aligned}}$$

6. If $C_1 < 0$:

$$Ab_3 = C_1 + Ab_2 \quad \text{else} \quad Ab_3 = Ab_2$$

$$Ns_1 = -C_1 \quad \text{else} \quad Ns_1 = 0$$

$$\boxed{\begin{aligned} Ab_3 &= 0 \\ Ns_1 &= 0 \end{aligned}}$$

7. If $Ab_3 < 0$:

$$Ns_2 = Ab_2 \quad \text{else} \quad Ns_2 = Ns_1$$

$$Or_1 = C_1 + Ab_2 + Or_p \quad \text{else} \quad Or_1 = Or_p$$

$$Ks_1 = -C_1 - Ab_2 \quad \text{else} \quad Ks_1 = 0$$

$$\boxed{\begin{aligned} Ns_2 &= 0 \\ Or_1 &= 0.004777 \\ Ks_1 &= 0 \end{aligned}}$$

8. If $Il_1 > Fs_p$:

$$\left[\begin{aligned} Il_2 &= Fs_p \quad \text{else} \quad Il_2 = Il_1 \\ Fs_1 &= Fs_p - Il_2 \end{aligned} \right]$$

$$\text{if } Il_1 > Il_2, \quad Tn_1 = Il_1 - Il_2 \quad \text{else} \quad Tn_1 = 0$$

$$\text{if } Tn_1 > Wo_2, \quad Tn_2 = Wo_2 \quad \text{else} \quad Tn_2 = Tn_1$$

$$\text{if } Tn_2 < 0, \quad Tn_3 = 0 \quad \text{else} \quad Tn_3 = Tn_2$$

$$Ru_1 = Tn_1 - Tn_3$$

$$Wo_3 = Wo_2 - Tn_3$$

$$\text{if } Hm_2 < Fs_1, \quad Mt_1 = Hm_2 \quad \text{else} \quad Mt_1 = Fs_1$$

$$Fs_2 = Fs_1 - Mt_1$$

$$\text{if } (En_p + Fs_2) > Wo_3,$$
$$Hy_1 = (En_p + Fs_2) - Wo_3 \quad \text{else} \quad Hy_1 = 0$$

$$\text{if } Wo_3 > (En_p + Fs_2), \quad Di_1 = En_p + Fs_2$$
$$\text{else} \quad Di_1 = Wo_3$$

$$Wo_4 = Wo_3 - Di_1$$

$$\text{Il}_2 = 0.012145$$
$$\text{Fs}_1 = 0.784994$$
$$\text{Tn}_1 = 0$$
$$\text{Tn}_2 = 0$$
$$\text{Tn}_3 = 0$$
$$\text{Ru}_1 = 0$$
$$\text{Wo}_3 = 0$$
$$\text{Mt}_1 = 0$$
$$\text{Fs}_2 = 0.784994$$
$$\text{Hy}_1 = 0.7974$$
$$\text{Di}_1 = 0$$
$$\text{Wo}_4 = 0$$

9. Reset the provisional amount of the following minerals as follows:

$$\text{Or}_p = \text{Or}_1, \quad \text{Ab}_p = \text{Ab}_3, \quad \text{An}_p = \text{An}_1,$$

$$\text{Di}_p = \text{Di}_1, \quad \text{Hy}_p = \text{Hy}_1$$

$$\text{Ac}_p = \text{Ac}_2, \quad \text{Ks}_p = \text{Ks}_1, \quad \text{Ns}_p = \text{Ns}_2,$$

$$\text{Wo}_p = \text{Wo}_4, \quad \text{Tn}_p = \text{Tn}_3$$

$$\text{Or}_p = 0.004777, \ \text{Ab}_p = 0,$$
$$\text{An}_p = 0.066986,$$
$$\text{Di}_p = 0, \ \text{Hy}_p = 0.7974$$
$$\text{Ac}_p = 0, \ \text{Ks}_p = 0, \ \text{Ns}_p = 0,$$
$$\text{Wo}_p = 0, \ \text{Tn}_p = 0$$

10. Calculate provisional quartz as:

$$Q_1 = \text{SiO}_2 - (6\text{Or}_p + 6\text{Ab}_p + 2\text{An}_p + 2\text{Di}_p$$
$$+\text{Hy}_p + 4\text{Ac}_p + \text{Ks}_p + \text{Ns}_p + \text{Wo}_p + \text{Tn}_p)$$

$$\boxed{Q_1 = -0.493525}$$

11. If $Q_1 < 0$:

$$\text{Ol}_1 = -Q_1 \quad \text{else} \quad \text{Ol}_1 = 0$$

$$\text{Hy}_2 = 2Q_1 + \text{Hy}_p$$

$$\boxed{\begin{array}{l} \text{Ol}_1 = 0.493525 \\ \text{Hy}_2 = -0.189649 \end{array}}$$

12. If $\text{Hy}_2 < 0$:

$$\text{Pf}_1 = \text{Tn}_p + \text{Hy}_2 \quad \text{else} \quad \text{Pf}_1 = 0$$

$$\text{if } \text{Pf}_1 < 0, \quad \text{Pf}_2 = \text{Tn}_p \quad \text{else} \quad \text{Pf}_2 = \text{Pf}_1$$

$$\text{Tn}_4 = \text{Tn}_p - \text{Pf}_2$$

$$Q_2 = Q_1 + \text{Pf}_2$$

$$\boxed{\begin{array}{l} \text{Pf}_1 = -0.189649 \\ \text{Pf}_2 = 0 \\ \text{Tn}_4 = 0 \\ Q_2 = -0.493525 \end{array}}$$

13. If $Q_p < 0$:

$$\text{Ol}_2 = -Q_2 \quad \text{else} \quad \text{Ol}_2 = 0$$

$$\text{Hy}_3 = 2Q_2 + \text{Hy}_p$$

$$\boxed{\begin{array}{l} \text{Ol}_2 = 0.493525 \\ \text{Hy}_3 = -0.189649 \end{array}}$$

14. If $\text{Hy}_3 < 0$:

$$\text{Ol}_3 = 0.5\text{Hy}_p \quad \text{else} \quad \text{Ol}_3 = \text{Ol}_2$$

$$\text{Ne}_1 = -0.25Q_2 - 0.125\text{Hy}_p \quad \text{else} \quad \text{Ne}_1 = 0$$

$$\text{Ab}_4 = 0.25Q_2 + 0.125\text{Hy}_p + \text{Ab}_p$$

$$\text{else} \quad \text{Ab}_4 = \text{Ab}_p$$

$$\boxed{\begin{array}{l} \text{Ol}_3 = 0.3987 \\ \text{Ne}_1 = 0.023706 \\ \text{Ab}_4 = -0.023706 \end{array}}$$

15. If $Ab_4 < 0$:

$$Ne_2 = Ab_p \quad \text{else} \quad Ne_2 = Ne_1$$

$$Lc_1 = -0.5Q_2 - 0.25Hy_p - 2Ab_p$$

$$\text{else} \quad Lc_1 = 0$$

$$Or_2 = 0.5Q_2 + 0.25Hy_p + 2Ab_p + Or_p$$

$$\text{else} \quad Or_2 = Or_p$$

$$\boxed{\begin{array}{l} Ne_2 = 0 \\ Lc_1 = 0.474124 \\ Or_2 = -0.042635 \end{array}}$$

16. If $Or_2 < 0$:

$$Lc_2 = Or_p \quad \text{else} \quad Lc_2 = Lc_1$$

$$Cs_1 = -Q_2 - 0.5Hy_p - 4Ab_p - 2Or_p$$

$$\text{else} \quad Cs_1 = 0$$

$$Wo_5 = 2Q_2 + Hy_p + 8Ab_p + 4Or_p + Wo_p$$

$$\text{else} \quad Wo_5 = Wo_p$$

$$\text{if } Wo_5 < 0, \quad Cs_2 = 0.5Wo_p \quad \text{else} \quad Cs_2 = 0$$

$$\boxed{\begin{array}{l} Lc_2 = 0.004777 \\ Cs_1 = 0.085270 \\ Wo_5 = -0.17054 \\ Cs_2 = 0 \end{array}}$$

17. If $Wo_5 < 0$:

$$Ol_4 = -0.5Q_2 + 0.25Hy_p - 2Ab_p - Or_p$$

$$\text{else} \quad Ol_4 = Ol_3$$

$$Cs_3 = Cs_2 - 0.5Q_2 - 0.25Hy_p - 2Ab_p - Or_p$$

$$\text{else} \quad Cs_3 = Cs_1$$

$$Di_2 = Q_2 + 0.5Hy_p + 4Ab_p + 2Or_p + Di_p$$

$$\text{else} \quad Di_2 = Di_p$$

$$\boxed{\begin{array}{l} Ol_4 = 0.441335 \\ Cs_3 = 0.042635 \\ Di_2 = -0.08527 \end{array}}$$

18. If $Di_2 < 0$:

$$Ol_5 = 0.5Hy_p + 0.5Di_p \quad \text{else} \quad Ol_5 = Ol_4$$

$$Lc_3 = 0.5Q_2 + 0.25Hy_p + 2Ab_p + 2Or_p$$

$$+ 0.5Di_p \quad \text{else} \quad Lc_3 = Lc_1$$

$$Cs_4 = 0.5Di_p + Cs_2 \quad \text{else} \quad Cs_4 = Cs_3$$

$$Kp_1 = -0.5Q_2 - 0.25Hy_p - 2Ab_p - Or_p$$

$$- 0.5Di_p \quad \text{else} \quad Kp_1 = 0$$

$$\boxed{\begin{array}{l} Ol_5 = 0.3987 \\ Lc_3 = -0.03786 \\ Cs_4 = 0 \\ Kp_1 = 0.042635 \end{array}}$$

19. If $Lc_3 < 0$:

$$Lc_4 = 0 \quad \text{else} \quad Lc_4 = Lc_2$$

$$Kp_2 = Lc_2 \quad \text{else} \quad Kp_2 = Kp_1$$

$$\text{if both } (Lc_3 > 0) \quad \text{and} \quad (Kp_2 > 0),$$

$$Lc_5 = Lc_3 \quad \text{else} \quad Lc_5 = Lc_4$$

$$\boxed{\begin{array}{l} Lc_4 = 0 \\ Kp_2 = 0.004777 \\ Lc_5 = 0 \end{array}}$$

20. This step is an extension to the classic CIPW norm calculation and takes care of the residual SiO_2 deficiency, if any, existing even after the formation of Kp by the breakdown of Lc.

$$Q_3 = 2(Kp_2 - Kp_1)$$

$$\text{if } C_p < 0, \quad C_2 = 0 \quad \text{else} \quad C_2 = C_p$$

$$Cs_5 = Cs_4 - \frac{1}{3}Q_3$$

$$C_3 = -\frac{2}{3}Q_3$$

$$An_2 = An_p + \frac{2}{3}Q_3$$

$$\boxed{\begin{array}{l} Q_3 = -0.075716 \\ C_2 = 0.005128 \\ Cs_5 = 0.025238 \\ C_3 = 0.050477 \\ An_2 = 0.016509 \end{array}}$$

21. Assign molecular fractions to the normative minerals as follows:

if $Q_2 < 0$, $Q = 0$ else $Q = Q_2$

if $Or_2 < 0$, $Or = 0$ else $Or = Or_2$

if $Ab_4 < 0$, $Ab = 0$ else $Ab = Ab_4$

if $Di_2 < 0$, $Di = 0$ else $Di = Di_2$

if $Hy_3 < 0$, $Hy = 0$ else $Hy = Hy_3$

if $Wo_5 < 0$, $Wo = 0$ else $Wo = Wo_5$

$C = C_2 + C_3$, $An = An_2$, $Ne = Ne_2$, $Ol = Ol_5$, $Mt = Mt_1$

$Il = Il_2$, $Ap = Ap_1$, $Ac = Ac_p$, $Lc = Lc_5$, $Ks = Ks_1$, $Ns = Ns_2$

$Cs = Cs_5$, $Kp = Kp_2$, $Hm = Hm_2$, $Tn = Tn_4$, $Ru = Ru_1$

$Pf = Pf_2$, $Cc = Cc_1$, $Py = Py_1$, $Cm = Cm_1$, $Fr = Fr_1$, $Z = Z_1$

$$\boxed{\begin{array}{l} Q = 0 \\ Or = 0 \\ Ab = 0 \\ Di = 0 \\ Hy = 0 \end{array}}$$

$$\boxed{\begin{array}{l} Wo = 0 \\ C = 0.0556055, \ An = 0.016509, \\ Ne = 0, \ Ol = 0.3987, \ Mt = 0 \\ Il = 0.012145, \ Ap = 0.000916, \\ Lc = 0, \ Ks = 0, \quad Ns = 0 \\ Cs = 0.025238, \ Kp = 0.004777, \\ Hm = 0, \ Tn = 0, \quad Ru = 0 \\ Pf = 0, \ Cc = 0, \ Py = 0, \ Cm = 0, \\ Fr = 0, \ Z = 0 \end{array}}$$

22. Calculate the formula weights of the normative minerals using the molecular weights of the oxides. For FeO and CaO use the molecular weights determined as follows:

$$\text{Mol wt. FeO} = \frac{\text{Wt.\%(FeO + MnO + NiO)}}{\text{Moles(FeO + MnO + NiO)}}$$

$$\text{Mol wt. CaO} = \frac{\text{Wt.\%(CaO + BaO + SrO)}}{\text{Moles(CaO + BaO + SrO)}}$$

$$\boxed{\begin{array}{l} \text{Mol wt. FeO} = 71.8444 \\ \text{Mol wt. CaO} = 56.0774 \end{array}}$$

23. Estimate the formula weights of the ferromagnesian minerals hypersthene, diopside and olivine as follows:

$$\text{Fraction Fe} = \frac{Fs_2}{(En_p + Fs_2)}$$

$$\text{Fraction Mg} = \frac{En_p}{(En_p + Fs_2)}$$

Formula wt. Hy = Fraction Mg $\times$ Mol wt. En
$\qquad$ + Fraction Fe $\times$ Mol wt. Fs

Formula wt. Di = Formula wt. Hy
$\qquad$ + Mol wt. Wo

Formula wt. Ol = Fraction Mg $\times$ (Mol wt. En
$\qquad$ + Mol wt. MgO) + Fraction Fe
$\qquad$ $\times$ (Mol wt. Fs + Mol wt. FeO)

Fraction Fe = 0.984442

Fraction Mg = 0.015558

Formula wt. Hy = 131.438

Formula wt. Di = 247.5997

Formula wt. Ol = 202.7917

24. Determine the weight percentages of the normative minerals by multiplying their molecular fractions with respective formula weights.

C = 5.669607, An = 4.592971,

Ol = 80.85302

Il = 1.842577, Ap = 0.923732

Cs = 4.347064, Kp = 1.511175

25. Find the sum of the weight percentages of normative minerals. Add to it

$$\text{Moles}(\text{Py} + \text{Fr} + \text{Ap}) \times 15.9994$$

$$- (\text{Moles Ap} \times 2 + \text{Moles Fr}) \times 18.9984$$

$$+ \text{Atoms F} \times 18.9984 + \text{Moles Cs}_2 \times 60.0843$$

where 15.9994 = At. wt. O, 18.9984 = At. wt. F, 60.0843 = Mol. wt. SiO_2. This sum should exactly match with the sum of the weight percentages of the oxides. Sum of the weights of the normative minerals is 99.74015. Because no pyrite or fluorite are in the norm; the first and second terms in the correction above become Moles Ap × 15.9994 − Moles Ap × 2 × 18.9984 = 0.000916 × 15.9994 − 0.000916 × 2 × 18.9984 = −0.02015. Because there was no fluorine in the input and Cs_2 is zero as determined in step 16, the rest two terms amount to zero. Therefore, the corrected sum of the normative minerals will be 99.74015 − 0.02015 = 99.72000.

Sum (oxides) = 99.72

Sum (normative minerals) = 99.74015

Corrected sum (normative minerals) = 99.72

The result is summarized below. Note that the effect of partitioning the total Fe between Fe^{2+} and Fe^{3+} is given in the columns numbered 2. The equation of Le Maitre (1976) has been used as the composition falls beyond the limits of the TAS diagram.

	Oxides (wt. %)	
	1	2
SiO_2	28.03	27.79
TiO_2	0.97	0.96
Al_2O_3	7.84	7.77
Fe_2O_3	0.00	11.47
FeO	57.27	46.45
MgO	0.50	0.50
CaO	4.27	4.23
K_2O	0.45	0.45
P_2O_5	0.39	0.39
Total	99.72	100.00
	Norms (wt. %)	
	1	2
C	5.66961	0.51834
Or	0.00000	2.63616
An	4.59297	18.47367
Hy	0.00000	3.60070
Ol	80.85302	55.42251
Mt	0.00000	16.62639
Il	1.84258	1.82652
Ap	0.92373	0.91568
Cs	4.34706	0.00000
Kp	1.51118	0.00000
Total	99.74015	100.01997
Corrected total	99.72000	100.00000

4. Causes of mass discrepancy

In the calculation of the CIPW norm, we start with definite amounts of different oxides and get at the end a set of minerals of definite quantities that can be formed by consuming these oxides. It is but natural that the weights of the oxides and that of the normative minerals should be the same, but it rarely happens so. Norms calculated from the same set of oxides in same quantities using different approaches do not always have identical values. Assuming all methods correctly estimate the norm, this kind of discrepancy can arise from the fact that different people use slightly different values for the oxide molecular weights. Sticking to a standard set of molecular weights would be preferable for achieving a standard norm.

The difference between the totals of the oxides and that of the minerals may arise due to a lack of internal consistency in the implemented steps of calculation. The calculation procedure may not be working as expected in different composition ranges. A logically simple and easy to understand formulation of the calculation procedure is therefore desirable.

Once all logical and computational errors are dealt with, mass discrepancy can arise due to three causes. Firstly, corrected molecular weights of FeO and CaO need to be used because of the fact that moles of MnO and NiO are added to FeO, and moles of BaO and SrO are added to CaO. Corrected molecular weight of FeO can be easily estimated by dividing the sum of weights of FeO, MnO and NiO by the sum of the molecular fractions of the three. Corrected molecular weight of CaO can be similarly estimated. The second cause of discrepancy is because the mineral formulas of pyrite (FeS_2), fluorite (CaF_2) and apatite ($9CaO \cdot 3P_2O_5 \cdot CaF_2$) are defined partially or completely by chemical species other than oxides, whereas all chemical constituents are input in the form of oxides. The discrepancy, for example, in the case of pyrite can be removed if we calculate the formula weight of pyrite as mol.wt.(FeO) + at.wt.(S) $\times$ 2 instead of as at.wt.(Fe) + at.wt.(S) $\times$ 2. Appropriate corrections in the sum of the mineral weights should be applied to take care of this discrepancy if true formula weights are used. The third source of mass discrepancy is from significant rounding off errors. The only scope of introducing significant rounding off error in the procedure delineated above is in the 20th step. Care must be taken to avoid using 0.333333... in place of 1/3 and 0.666666... in place of 2/3 which can result in considerable mismatch between the sums in some cases.

If all Wo is converted to Cs in step 16, an equivalent amount of SiO_2 must be added to the final sum.

Finally, it is to be noted that this budgeting exercise is just unnecessary as it has no effect on the calculated norms. However, it works as a beautiful check against inconsistencies in the input values and provides a guard against unsuspected errors.

5. Discussion

Although trace element and isotope geochemistry have surpassed the CIPW norm in the interpretation of igneous rocks, the role of CIPW norm remains unbeaten in the use of it in the classification of igneous rocks, that of the volcanic rocks in particular. Very precise discriminative parameters used in the classification of the igneous rocks demand for very precise calculation of the CIPW norm. There are a number of superior computer packages available for petrological purpose (Petro-Graph, GeoPlot and SINCLAS, to name a few), but none of them reproduce the total of the oxides to the degree required. SINCLAS (Verma *et al* 2002), for example, even after using simplified calculation method of Kelsey (1965) and using variable atomic weights, has an inaccuracy of up to 0.002% m/m (wt.%). The new set of rules presented here use easy to understand linear algebraic equations and so, minimize the chance of error in the estimation of the normative minerals. Further, the steps for calculation of the norm are given in a programmer-friendly manner removing the scope of any ambiguity. Possible error due to the presence of SiO_2 deficiency beyond the scope of the classic scheme of calculation has been preempted by introducing additional steps for calculation and steps to prevent erroneous estimation of the sum of the normative minerals have been provided. The method has been checked for about 11,200 analyses spanning a wide variety of rocks. A comparison with the results obtained from SINCLAS shows that there is insignificant difference between the calculated norms. However, with the present calculation scheme all factors contributing towards differences between the total of the analyses and the total of the norms have been completely resolved. For example, the norms for an ultrabasic rock analysis have been compared below with the results obtained from SINCLAS. When rounded to the third decimal place, norms compare well except for apatite. This difference is because of the fact that the formula for apatite in the present scheme is uniformly taken as $9CaO \cdot 3P_2O_5 \cdot CaF_2$ (equivalent to $3CaO \cdot P_2O_5 \cdot 1/3CaF_2$) whether or not F is there in the input and the final sum of the normative minerals are corrected accordingly. The

	Oxide (wt%)		Norm (wt.%)	
			Present study	SINCLAS
SiO_2	44.906	Or	1.81426	1.814
TiO_2	2.709	Alb	15.56949	15.569
Al_2O_3	14.945	An	31.61230	31.612
Fe_2O_3	1.927	Di	16.47141	16.471
FeO	12.850	Hy	7.62915	7.629
MnO	0.215	Ol	18.13576	18.135
MgO	9.057	Mt	2.79378	2.794
CaO	10.887	Il	5.14541	5.145
Na_2O	1.840	Ap	0.83197	0.829
K_2O	0.307			
P_2O_5	0.358			
Total	100.001	Total	100.00352	99.998
		Corrected total	100.00100	

uncorrected sum of the normative minerals according to the proposed scheme is closer to the sum of the oxides with a difference of $+0.00252$ whereas SINCLAS has a difference of -0.00300. The corrected total of the normative minerals as suggested in step 25 and explained in the previous section completely takes care of this difference.

The method described here keeps clear of the issue of the standardization of the oxidation ratio (Fe_2O_3/FeO) of igneous rocks. The user should use his discretion to choose a scheme preferable to him. It is also left to the user as to whether the input analysis should be recast to 100% total or not. These decisions are crucial as they potentially alter the final norms obtained. For example, norms obtained from analysis recast to a total of 100% will be different from the final norm that has been recast to 100% total, obtained without normalizing the input analysis. For the sake of oxidation ratios, Verma *et al* (2002, 2003) suggest three options, but favour the method of Middlemost (1989). Whenever possible, actual analyses of Fe_2O_3 and FeO should be used to fix this ratio (Le Bas *et al* 1986), but keeping in mind the possibility of post-emplacement oxidation. Alternatively, the equation of Le Maitre (1976),

$$\frac{FeO}{FeO + Fe_2O_3} = 0.93 - 0.0042SiO_2$$

$$- 0.022(Na_2O + K_2O)$$

can be used to estimate the $FeO/(FeO + Fe_2O_3)$ ratio from which the Fe_2O_3/FeO ratio can be calculated. For example, if $FeO/(FeO + Fe_2O_3) = 0.869565$, $Fe_2O_3/FeO = (1/0.869565) - 1 = 0.15$. According to the method of Middlemost (1989), the Fe_2O_3/FeO ratio is fixed based on the rock type represented by the analysis. Verma *et al* (2002) superpose these values on the modified total alkali *vs.* silica (TAS) diagram (after Le Bas *et al* 1986; Le Bas 1989, 2000) which can be conveniently referred to for determining the Fe_2O_3/FeO ratio. Note that for using the Middlemost method it is required to recalculate the analysis on a volatile free 100% total basis.

Once the Fe_2O_3/FeO ratio is fixed according to the method of either Le Maitre (1986) or of Middlemost (1989), the FeO and Fe_2O_3 amounts in the analysis can be adjusted as follows. Convert all FeO to Fe_2O_3 as $Fe_2O_3 = FeO \times 1.111348$ and add this amount to the already existing Fe_2O_3, if any. If $Fe_2O_3/FeO = R$,

$$FeO_{Adjusted} = \left(\frac{(Fe_2O_3)_{Total}}{1 + R \times 0.899809}\right) \times 0.899809$$

and

$$(Fe_2O_3)_{Adjusted} = (Fe_2O_3)_{Total} - \left(\frac{(Fe_2O_3)_{Total}}{1 + R \times 0.899809}\right).$$

Most up-to-date atomic weights of elements recommended by the IUPAC Commission on Atomic weights and Isotopic Abundances (Vocke 1999) have been used for the calculation of molecular weights of the oxides and the formula weights of the normative phases. For obtaining standard norms, this is important. Two calculation schemes, although being perfectly correct in their respective methodologies, will yield different norms just because they may be using different sets of atomic weights. Because SINCLAS uses the same atomic weights, it was possible to compare the results obtained from the present scheme with that obtained from SINCLAS. The present scheme failed to calculate in case of 12 analyses out of the approximately 11,200 analyses used to check its efficacy. In these analyses $1/3$(moles P_2O_5) exceeded $1/10$(moles CaO). Because all P_2O_5 is assigned to apatite, CaO falls short in these analyses. Such inconsistencies in the input data should be removed before the calculation of the norm is attempted.

6. Conclusions

Present study suggests a set of simple equations for the calculation of CIPW norms for igneous rocks. These equations are obtained by simultaneous solution by matrix methods of a set of equations representing either the breakdown of the Al_2O_3-saturated minerals to their Al_2O_3-undersaturated counterparts or that of the SiO_2-saturated minerals to their SiO_2-undersaturated counterparts. The use of these equations for the calculation of the CIPW norm is implemented through 25 programmer-friendly steps. Use of modified molecular weights for CaO and FeO, corrected formula weights for apatite and pyrite, and measures taken to avoid significant rounding off errors at step number 20 achieve complete removal of mass discrepancies between the totals of the oxides and the totals of the normative minerals. A database consisting of a worldwide compilation of about 11,200 analyses from a large number of publications that were compiled and periodically updated by the following workers: Pal *et al* (1978); Aguilar-Y-Vargas and Verma (1987); Verma (2000, 2002, 2004, 2006); Agrawal *et al* (2004, 2008); Verma *et al* (2006) and Agrawal and Verma (2007) provided representative

rock chemistry data for an objective evaluation of the functioning of the algorithm presented here. See these papers for more complete list of references. The results completely agree except for apatite, as far as the norms are concerned, with the results obtained from the most recent, precise and accurate computer program SINCLAS of Verma *et al* (2002, 2003). Additionally, an absolute match between the totals of the oxides and the norms, which eluded all earlier schemes of norm calculation, is achieved in the present study.

Acknowledgements

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