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Contributions to Mineralogy and Petrology

Corrections to expressions for calculating mineral components in "Origin of Calc-Alkaline Series Lavas at Medicine Lake Volcano by Fractionation, Assimilation and Mixing" and "Experimental Petrology of normal MORB near the Kane Fracture Zone: 22°–25°N, mid-Atlantic ridge"

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The purpose of this note is to point out errors that were introduced in presenting the expressions for the recalculation of liquid and mineral compositions into mineral components discussed by Grove et al. (1982, 1983) and in Tormey et al. (1987). In both papers there are errors in one of the equations used in the recalculation scheme. This correction describes the method of recalculation and provides the correct expressions for the Tormey et al. (1987) and Grove et al. (1982) projection schemes. The errors in the Grove et al. (1982) and Tormey et al. (1987) equations do not affect the conclusions drawn in either of the papers. The incorrect equations were introduced during manuscript preparation and overlooked by myself during final editing. These errors have been brought to my attention by individuals who have tried to use the projection schemes over the past few years. I have supplied and will continue to provide interested individuals with a FORTRAN program that calculates the mineral components from chemical analyses expressed in weight % oxides. I present the corrected expressions in this note, because interest in using these equations has continued and therefore a formal note discussing the corrections seemed appropriate.

The error in the projection calculation used by Grove et al. (1982, Fig. 3 caption) appeared in the Qtz expression, and in the correct expression Cr_2O_3 should be divided by 2 and TiO_2 has no multiplier. The error in Tormey et al. (1987, Fig. 4 caption) appeared in the Cpx equation where the term ($KO_{0.5}$–$NaO_{0.5}$) should be ($KO_{0.5}$+ $NaO_{0.5}$) or Alk in the equations below.

Recalculation procedure

First, recalculate the composition of the lava, liquid or mineral from weight % oxides into mole %. Next, recalculate Al_2O_3, Fe_2O_3, K_2O, Na_2O and P_2O_5 as $AlO_{1.5}$, $Fe^{3+}O_{1.5}$, $KO_{0.5}$, $NaO_{0.5}$ and $PO_{2.5}$. An example calculation that follows this procedure is provided in Table 1.

To transform to the mineral components of Grove et al. (1982) use the following expressions:

Table 1. A worked example of the Grove et al. (1982) mineral component transformation for composition 79–35 g #2 gl from Table 2 of Grove et al. (1982)

Weight % oxides									
SiO_2	TiO_2	Al_2O_3	Cr_2O_3	FeO	MgO	MnO	CaO	K_2O	Na_2O
50.70	1.83	13.30	0.01	12.50	7.06	0.21	11.5	0.11	1.47
Molar components									
53.43	1.45	8.26	0.0	11.02	11.09	0.19	12.98	0.07	1.50
Molar monoxide components									
48.65	1.32	15.04	0.0	10.03	10.10	0.17	11.82	0.13	2.73
Mineral component recalculation									
Sum	Qtz	Plag	Oliv	Cpx	Or	Sp			
0.3242	0.1055	0.0882	0.0588	0.0573	0.0013	0.0132			
Molar mineral components									
	0.325	0.272	0.181	0.177	0.004	0.041			
Oxygen units									
	0.135	0.453	0.151	0.221	0.007	0.034			

Table 2. Transformation of basis vectors from monoxide molar components to molar mineral components

	Minerals	Or	Ab	Chr	Usp	An	Di	Ol	Qtz
Oxides									
$KO_{0.5}$	=	1							
$NaO_{0.5}$	=	0	1						
Cr_2O_3	=	0	0	1					
TiO_2	=	0	0	0	1				
$AlO_{1.5}$	=	1	1	0	0	2			
CaO	=	0	0	0	0	1	1		
FMO	=	0	0	1	2	0	1	2	
SiO_2	=	3	3	0	0	2	2	1	1

Table 3. Equations for mineral components obtained by subtracting successive rows until only the elements of the leading diagonal contain non-zero terms. To renormalize the new components to unity, each expression on the left must be divided by the sum of the left-hand equations

									Or	Ab	Chr	Usp	An	Di	Ol	Qtz
$+KO_{0.5}$								=	1							
	$+NaO_{0.5}$							=		1						
		$+Cr_2O_3$						=			1					
			$+TiO_2$					=				1				
$-KO_{0.5}/2$	$-NaO_{0.5}/2$			$+AlO_{1.5}/2$				=					1			
$+KO_{0.5}/2$	$+NaO_{0.5}/2$			$-AlO_{1.5}/2$	$+CaO$			=						1		
$-KO_{0.5}/4$	$-NaO_{0.5}/4$	$-Cr_2O_3/2$	$-TiO_2$	$+AlO_{1.5}/4$	$-CaO/2$	$+FMO/2$		=							1	
$-11KO_{0.5}/4$	$-11NaO_{0.5}/4$	$+Cr_2O_3/2$	$+TiO_2$	$-AlO_{1.5}/4$	$-3CaO/2$	$-FMO/2$	$+SiO_2$	=								1

$$\text{Sum} = SiO_2 - CaO - 2*(KO_{0.5} + NaO_{0.5}) + Cr_2O_3 + TiO_2$$

$$\text{Qtz} = \{SiO_2 - 0.5*(FeO + MgO) - 1.5*CaO - 0.25*AlO_{1.5} - 2.75*(KO_{0.5} + NaO_{0.5}) + 0.5*Cr_2O_3 + TiO_2\}/\text{Sum}$$

$$\text{Plag} = \{0.5*(AlO_{1.5} + NaO_{0.5} - KO_{0.5})\}/\text{Sum}$$

$$\text{Oliv} = \{0.5*(FeO + MgO + 0.5*[AlO_{1.5} - KO_{0.5} - NaO_{0.5}] - CaO - 2*TiO_2 - Cr_2O_3)\}/\text{Sum}$$

$$\text{Cpx} = \{CaO - 0.5*AlO_{1.5} + 0.5*(KO_{0.5} + NaO_{0.5})\}/\text{Sum}$$

$$\text{Or} = \{KO_{0.5}\}/\text{Sum}$$

$$\text{Sp} = \{Cr_2O_3 + TiO_2\}/\text{Sum}$$

In the following, molar MgO and FeO have been combined into the component FMO and $KO_{0.5}$ and $NaO_{0.5}$ into the component Alk. To transform to the mineral components of Tormey et al. (1987) use the following expressions:

$$\text{Sum} = SiO_2 - CaO - 2*\text{Alk} + Cr_2O_3 + TiO_2 + 2*PO_{2.5} + FeO_{1.5}$$

$$\text{Qtz} = \{SiO_2 - 0.5*\text{FMO} - 1.5*CaO - 0.25*AlO_{1.5} - 2.75*\text{Alk} + 0.5*Cr_2O_3 + 0.5*TiO_2 + 2.5*PO_{2.5}\}/\text{Sum}$$

$$\text{Plag} = \{AlO_{1.5} + NaO_{0.5} - KO_{0.5}\}/\{2.0*\text{Sum}\}$$

$$\text{Oliv} = \{\text{FMO} + 0.5*(AlO_{1.5} - \text{Alk}) - CaO - TiO_2 - Cr_2O_3 + 1.667*PO_{2.5}\}/\{2.\ 0*\text{Sum}\}$$

$$\text{Cpx} = \{CaO - 0.5*AlO_{1.5} + 0.5*\text{Alk} - 1.667*PO_{2.5}\}/\text{Sum}$$

$$\text{Ilm-Hem-Chr} = \{Cr_2O_3 + TiO_2 + FeO_{1.5}\}/\text{Sum}$$

$$\text{Or} = KO_{0.5}/\text{Sum}$$

$$\text{Ap} = PO_{2.5}/\{3*\text{Sum}\}$$

These molar mineral components are then transformed to oxygen units by multiplying the molar value by the number of oxygens in the mineral component and renormalizing to unity. Relative to the 2 oxygens in quartz the oxygen-based values become:

$$\text{Qtz}_{oxy} = \text{Qtz}_{mol}$$

$$\text{Plag}_{oxy} = 4*\text{Plag}_{mol}$$

$$\text{Oliv}_{oxy} = 2*\text{Oliv}_{mol}$$

$$\text{Cpx}_{oxy} = 3*\text{Cpx}_{mol}$$

$$\text{IHC}_{oxy} = 1.5*\text{IHC}_{mol}$$

$$\text{Or}_{oxy} = 4*\text{Or}_{mol}$$

$$\text{Ap}_{oxy} = 6*\ \text{Ap}_{mol}$$

These projection schemes represent a transformation of basis vectors that may be carried out by writing down the mineral components in terms of the molar monoxide components. The basis set is shown in Table 2 for the Grove et al. (1982) projection scheme. The order of the new components (mineral units, rows) and old components (oxide units, columns) is chosen so that the mineral equations (rows) containing only one oxide unit appear at the top of the matrix. Then the mineral equations containing more than one oxide follow. The arrangement of rows and columns shown in Table 2 facilitates inversion of the matrix by Gaussian elimination (see Strang 1980, Chap. 1). Gaussian elimination involves subtracting successive rows until only the leading diagonal contains non-zero terms. Because the matrix in Table 2 is lower triangular, the matrix may be inverted by subtracting overlying rows from underlying rows. Table 3 shows the final inverted matrix. The new components are then normalized to unity by dividing each term by the sum of the mineral components. In any situation where one wishes to convert from one set of components (i.e. oxides) to another representation of composition space (mineral components) the process described above may be useful.

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