Flow Diagram for a Computer Program Designed to Calculate Igneous Molecular Norms

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This paper describes one important aspect of a project carried out under the direction of Professor Charles J. Vitaliano by Dr. Richard D. Harvey and the author at Indiana University from 1960 to 1962. The history and theory of ingneous normative mineral computation has been reviewed by Barth (1), and the capabilities and intricacies of its computer programming have been briefly discussed elsewhere (2). The primary purpose of this paper is to present the unpublished flow diagram for this computation in a form adaptable to any electronic digital computer or usable as a guide for manual norm computation instruction.

This flow diagram is the schematic representation of a mathematical sequence of operations that make possible the conversion of the chemical analysis of an igneous rock into the probable quantitative mineral assemblage for that rock. This conversion process, if done manually requires 12 subtractions, 27 additions, 34 multiplications, 39 divisions and 6 comparisons for the computation of just one silica-rich igneous rock. The molecular norm computation was programmed for the computer primarily to avoid the inevitable human error resulting from this tedious process; secondarily to save time if large numbers of norms were required. An experienced person requires in excess of 15 minutes to complete the operation manually (if no mistakes are made) whereas the electronic computer requires about 8 seconds per computation.

The flow diagram (Fig. 1) presented here is nothing more than a series of quasi-mathematical statements connected by lines to show the sequence of operations. The "mathematical language" used here is that used by programmers but readily understandable to the interested geologist with the aid of the following basic rules illustrated by operations shown in figure 1, step 2, and identification of abbreviations, listed in figure 2. Boxed statements are standard mathematical operations that result in the changing of a stored value (such as the cation percentage of calcium oxide) to a reduced value required to account for material used in the formation of calcite; eg: $Ca = Ca - C(O_2)$. Circled statements represent mathematical questions that decide which of two possible steps should now be taken; eg: $Fe^{++} - Ti < 0$? (is ferrous oxide minus titanium oxide less than zero?) If the decision is yes, (titanium oxide exceeds ferrous oxide), then the next mineral, ilmenite, must be formed on the basis of available ferrous oxide; if the decision is no, then ilmenite will be formed from titanium oxide. Read in and print out statements are the only other basic statements required for computer operation of this program.
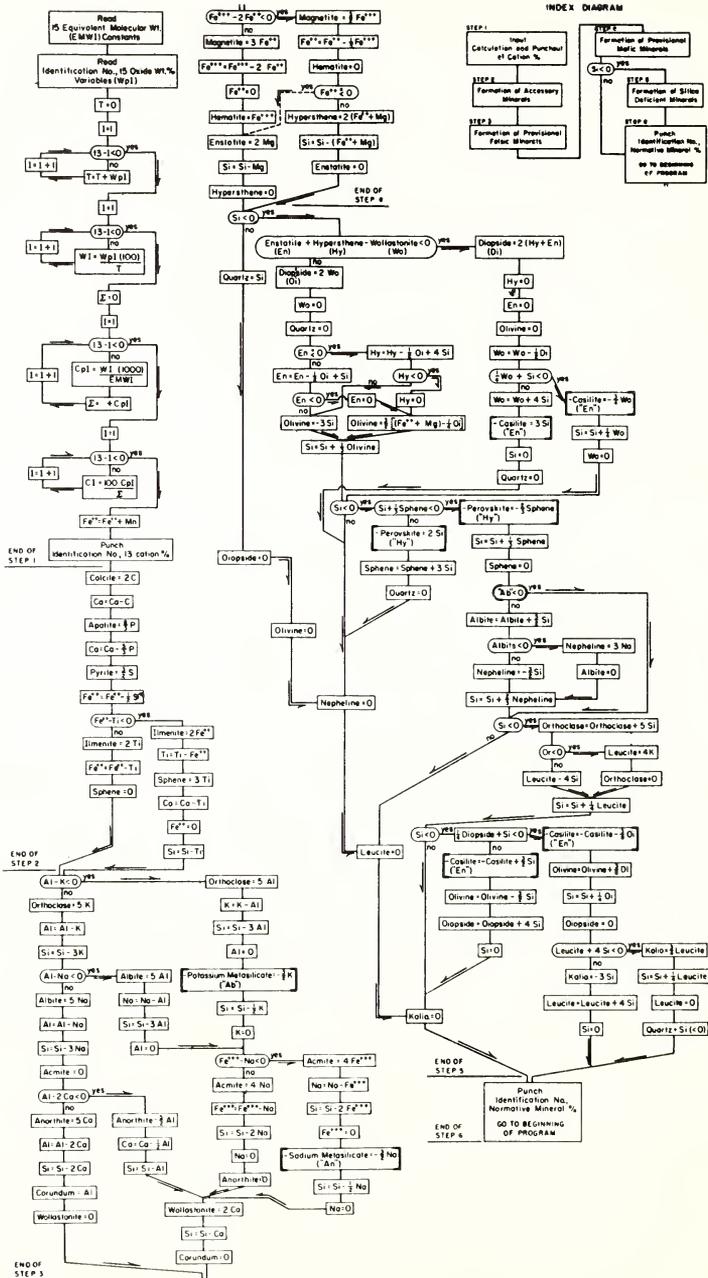
Figure 1.   Flow diagram for the computation of the molecular normative mineral assemblage of an igneous rock from oxide percentages obtained by chemical analysis.

Explanation

Direction of flow; downward if no arrow shown.
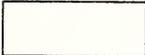
Performance of designated operation.

Performance of designated branching operation and flow directions.
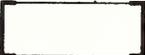
Operation involves formation of a silica deficient mineral, designated "X," that is stored in mineral location X as a negative value. Also indicated as

"Ab"	-Potassium Metasilicate ($-K_2SiO_3$)	K	$KO_{1/2}$
Al	$AlO_{3/2}$	Kalio.	Kaliophilite ($KAlSiO_4$)
"An"	-Sodium Metasilicate ($-Na_2SiO_3$)	Mg	MgO
C	CO_2	Mn	MnO
Ca	CaO	Na	$NaO_{1/2}$
CI	Cation % mineral I	Or	Orthoclase ($KAlSi_8$)
CpI	Cation proportion mineral I	P	$PO_{5/2}$
Di	Diopside ($CaMgSi_2O_6$)	S	Sulphur
EMWI	Equivalent Molecular Wt. Constant I	Si	SiO_2
En	Enstatite, ($MgSiO_3$)	T	Totals
"En"	-Casilite, ($-Ca_2SiO_4$)	Ti	TiO_2
Fe^{++}	FeO	WI	Adjusted wt. % I
Fe^{+++}	$FeO_{3/2}$	Wo	Wollastonite
Hy	Hypersthene $\left[(Mg, Fe)SiO_3\right]$	WpI	Chemical analysis wt. % I
"Hy"	-Perovskite ($-CaTiO_3$)	Σ	Sum
I	Index number	O	Zero

Figure 2.   Symbols and abbreviations used in the igneous norm flow diagram.

Literature Cited

1. BARTH, T. F. W. 1962. Theoretical Petrology. John Wiley and Sons, New York. 65-71.
2. VITALIANO, C. J., HARVEY, R. D. and CLEVELAND, J. H. 1965. Computer program for norm calculation. Amer. Minerologist **50**:495-498.