FORTRAN IV Computer Programme for Calculation of the Niggli Molecular Norm

CHARLES S. HUTCHISON
University of Malaya

JOHN E. JEACOCKE
University of Glasgow

Abstract: A complete FORTRAN IV computer programme has been devised for Niggli molecular norm calculations. It has been specifically designed for an I.B.M. 1130 computer, but can easily be modified for other versions of FORTRAN, or can be adapted to other programme languages.

INTRODUCTION

Norm calculation is a standard procedure for petrographers, as can be witnessed by the fact that publications which incorporate a table of rock chemical analyses usually also tabulate these analyses re-calculated as cationic percentages and as norms. All students of petrography have to struggle with the somewhat imprecise and often ambiguous rules for norm calculation, either using the C.I.P.W. system (Johannsen, 1939, pp. 88-92) or the Niggli method (Barth, 1962, pp. 65-70). The calculation is so monotonous and involved that seldom can identical results be obtained by different individual workers. This lack of reproducability, coupled with the time-consuming nature of the calculation, seems good reason for computerizing the norm calculation. We have devised a somewhat lengthy FORTRAN IV programme (I.B.M., 1964), which is designed specifically for an I.B.M. 1130 computer, such as the one in the Computer Centre of the University of Malaya, but it can easily be modified for other versions of FORTRAN, and adaptation to other programme languages is straightforward.

OUTLINE AND DESCRIPTION OF THE PROGRAMME

The programme, designated as NNorm (= Niggli norm), is designed to accept oxide analyses standardized in the following fixed order:

1. \( \text{SiO}_2 \)  2. \( \text{Al}_2\text{O}_3 \)  3. \( \text{TiO}_2 \)  4. \( \text{Fe}_2\text{O}_3 \)  5. \( \text{FeO} \)  6. \( \text{MnO} \)  7. \( \text{NiO} \)  8. \( \text{MgO} \)  9. \( \text{CaO} \)  10. \( \text{BaO} \)  11. \( \text{SrO} \)  12. \( \text{Na}_2\text{O} \)  13. \( \text{K}_2\text{O} \)  14. \( \text{P}_2\text{O}_5 \)  15. \( \text{CO}_2 \)  16. \( \text{ZrO}_2 \)  17. \( \text{F} \)  18. \( \text{S} \)  19. \( \text{Cr}_2\text{O}_3 \)  20. \( \text{Cl} \)  21. \( \text{SnO}_2 \)  22. \( \text{LiO}_2 \)  23. \( \text{CuO} \).

The amounts are listed in each case as 3 digits followed by two places after the decimal point, for example 36.21% is written as 03621. \( \text{H}_2\text{O}^+ \) and \( \text{H}_2\text{O}^- \) and any other oxides not included in the above list are omitted from the calculation and hence
from the tabulation. Determinations such as 'trace' and 'not determined' must be listed as 00000 in each case. The complete rock analysis is punched on 2 data cards using all columns continuously from 1 to 80 on the first card, according to the following scheme: SiO₂ occupies columns 1 to 5, Al₂O₃ 6 to 10, TiO₂ 11 to 15, ... ZrO₂ 76 to 80; then continuing on the second card, F occupying columns 1 to 5, and ending on columns 31 to 35 occupied by CuO.

A form such as shown in figure 1 has been designed for entering the chemical analysis in a way convenient for transferring to data cards.

![Figure 1](image-url)  
**Fig. 1.** Recommended form for tabulating the chemical analyses.

The programme has been designed to calculate and tabulate the normative minerals listed in Table 1. In constructing the programme, the rules of Barth (1962) have

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Abbreviation</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>quartz</td>
<td>QTZ</td>
<td>SiO₂</td>
</tr>
<tr>
<td>corundum</td>
<td>COR</td>
<td>Al₂O₃</td>
</tr>
<tr>
<td>zircon</td>
<td>ZIR</td>
<td>ZrO₂, SiO₂</td>
</tr>
<tr>
<td>orthoclase</td>
<td>OR</td>
<td>KO₁, AlO₁₂, 3SiO₂</td>
</tr>
<tr>
<td>albite</td>
<td>AB</td>
<td>NaO₃, AlO₁₂, 3SiO₂</td>
</tr>
<tr>
<td>anorthite</td>
<td>AN</td>
<td>CaO, 2AlO₁₂, 2SiO₂</td>
</tr>
<tr>
<td>leucite</td>
<td>LC</td>
<td>KO₁, AlO₁₂, 2SiO₂</td>
</tr>
<tr>
<td>nepheline</td>
<td>NE</td>
<td>NaO₃, AlO₁₂, SiO₂</td>
</tr>
<tr>
<td>kaliophilithe</td>
<td>KP</td>
<td>KO₁, AlO₁₂, SiO₂</td>
</tr>
<tr>
<td>halite</td>
<td>HL</td>
<td>NaCl</td>
</tr>
<tr>
<td>plagioclase</td>
<td>PLAG</td>
<td>AB₂+AN = AB₂AN₁₀₀−₄₆</td>
</tr>
<tr>
<td>acmite</td>
<td>AC</td>
<td>NaO₃, FeO₁₂, 2SiO₂</td>
</tr>
<tr>
<td>sodium metasilicate</td>
<td>NS</td>
<td>2NaO₁₂, SiO₂</td>
</tr>
<tr>
<td>potassium metasilicate</td>
<td>KS</td>
<td>2KO₃, SiO₂</td>
</tr>
</tbody>
</table>

---

Table 1. List of the normative minerals used in the programme.
(Table 1 continued)

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Abbreviation</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>wollastonite</td>
<td>WO</td>
<td>CaO, SiO₂</td>
</tr>
<tr>
<td>enstatite</td>
<td>EN</td>
<td>MgO, SiO₂</td>
</tr>
<tr>
<td>ferrosilite</td>
<td>FS</td>
<td>FeO, SiO₂</td>
</tr>
<tr>
<td>forsterite</td>
<td>FO</td>
<td>2MgO, SiO₂</td>
</tr>
<tr>
<td>fayalite</td>
<td>FA</td>
<td>2FeO, SiO₂</td>
</tr>
<tr>
<td>calcium orthosilicate</td>
<td>CS</td>
<td>2CaO, SiO₂</td>
</tr>
<tr>
<td>magnetite</td>
<td>MT</td>
<td>FeO, 2FeO₁₁₂</td>
</tr>
<tr>
<td>chromite</td>
<td>CM</td>
<td>FeO, 2CrO₁₂</td>
</tr>
<tr>
<td>hematite</td>
<td>HM</td>
<td>FeO₂</td>
</tr>
<tr>
<td>ilmenite</td>
<td>IL</td>
<td>FeO, TiO₂</td>
</tr>
<tr>
<td>titanite</td>
<td>TN</td>
<td>CaO, TiO₂, SiO₂</td>
</tr>
<tr>
<td>perovskite</td>
<td>PF</td>
<td>CaO, TiO₂</td>
</tr>
<tr>
<td>rutile</td>
<td>RU</td>
<td>TiO₂</td>
</tr>
<tr>
<td>apatite</td>
<td>AP</td>
<td>9CaO, 6PO₁₂, CaF₂</td>
</tr>
</tbody>
</table>

If there is no fluorine in the analysis, then AP = 5CaO, 3PO₁₂

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Abbreviation</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>fluorite</td>
<td>FR</td>
<td>CaF₂</td>
</tr>
<tr>
<td>pyrite</td>
<td>PR</td>
<td>FeS₂</td>
</tr>
<tr>
<td>calcite</td>
<td>CC</td>
<td>CaO, CO₂</td>
</tr>
<tr>
<td>cassiterite</td>
<td>CT</td>
<td>SnO₂</td>
</tr>
<tr>
<td>diopside</td>
<td>DI</td>
<td>WO₅₅EN₅₅FS₀₋ₓ</td>
</tr>
<tr>
<td>hypersthene</td>
<td>HY</td>
<td>EN₅₅EN₅₅FS₀₋ₓ</td>
</tr>
<tr>
<td>olivine</td>
<td>OL</td>
<td>FO₁₀₀FA₁₀₀₋ₓ</td>
</tr>
</tbody>
</table>

been followed, but expanded considerably to allow for all the additional minerals listed by Johannsen (1939). In addition, cassiterite has been added to cater for the high frequency of SnO₂ in Malayan rocks.

The programme occupies 397 I.B.M. cards, but can more conveniently be stored on magnetic disk, so that only the two control cards ('//JOB' and '//XEQ NNORM') are necessary to precede the pairs of data cards for each analysis. The final card has a 9 punched in column 1 only.

RESULTS

A specimen output of the computer programme is illustrated in figure 2. The abbreviations and layout are self-explanatory. The specimen selected for this illustration is a dolerite from near Kuala Suage Chempedak, Pahang, Malaya (Alexander, 1964, pp. 38-39, specimen 02.5.003). In addition to the tabulated data, H₂O⁺ is 2.46 and H₂O⁻ is 0.32. NiO is recorded as 'trace' and SrO, SnO₂, LiO₂ and CuO are not determined, hence all are tabulated as zero.

Cation percentages have been included in the output for the purpose of constructing variation diagrams. Diopside, hypersthene, olivine, and plagioclase are totalled and listed as molecular percentages of the respective end-members. Finally quartz, orthoclase, and plagioclase are re-calculated for plotting on triangular percentage diagrams.

The execution time on a 3.6 microsecond-cycle 1130 computer is 30 seconds for each set of data.

As far as can be checked, the programme is accurately set, and results check excellently with many examples which have been carefully calculated 'manually' by staff and students. Any discrepancies in the results have always been shown to result from the human element.
On very rare occasions, it has been found that anorthite (AN) is given as a negative value. Such cases result from insufficient CaO in the chemical analysis to combine both with the P₂O₅ to form apatite and with the CO₂ to form calcite. No suitable rule can be established for this situation, since it probably represents a faulty chemical analysis. We recommend, however, that when anorthite is given a negative value, then the norm be recalculated omitting either or both of CO₂ and P₂O₅ as necessary to allow AN to remain positive.

SUMMARY

This article is published to bring to the attention of petrographers and mineralogists the existence of a comprehensive workable FORTRAN IV computer programme for Niggli molecular norm calculations. A copy of the complete programme will be made available, upon request, from either one of the authors or from the editor of this bulletin. The geology department of the University of Malaya is willing to compute norms for petrographers who do not have access to a computer, provided the chemical analyses are submitted in the format of figure 1.
ACKNOWLEDGEMENT

We are grateful to the director of the Computer Centre of the University of Malaya for freely making the facilities available to us.

REFERENCES


