SHORT NOTES:

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# FORTRAN IV Computer Programme for Calculation of the Niggli Molecular Norm

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**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 reproducibility, 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

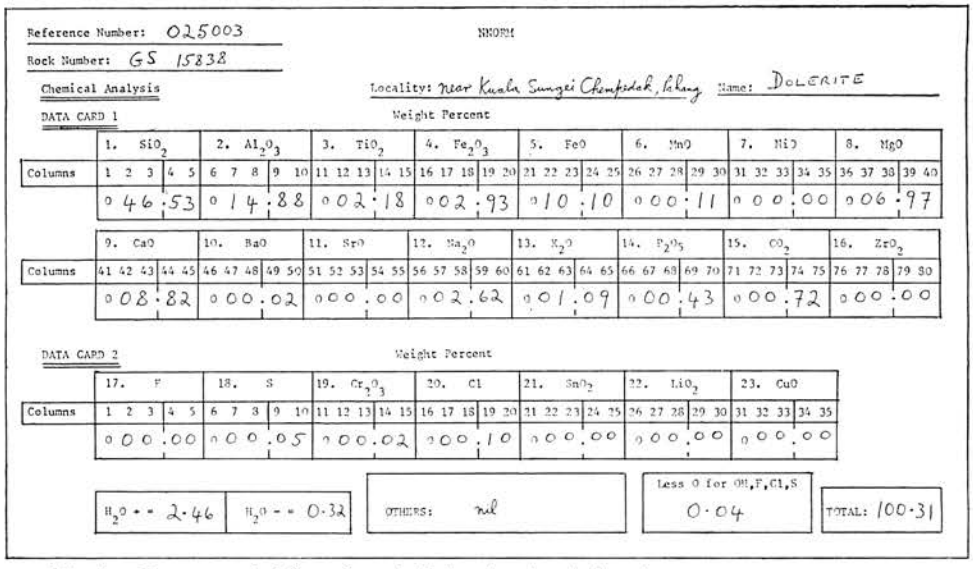
The programme, designated as NNORM (= Niggli norm), is designed to accept oxide analyses standardized in the following fixed order:

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1. | $SiO_2$ | 2. | $Al_2O_3$ | 3. | $TiO_2$ | 4. | $Fe_2O_3$ | 5. | FeO | 6. | MnO | 7. | NiO |
| 8. | MgO | 9. | CaO | 10. | BaO | 11. | SrO | 12. | $Na_2O$ | 13. | $K_2O$ | 14. | $P_2O_5$ |
| 15. | $CO_2$ | 16. | $ZrO_2$ | 17. | F | 18. | S | 19. | $Cr_2O_3$ | 20. | Cl | 21. | $SnO_2$ |
| 22. | $LiO_2$ | 23. | 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. $H_2O+$ and $H_2O-$ 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: $SiO_2$ occupies columns 1 to 5, $Al_2O_3$ 6 to 10, $TiO_2$ 11 to 15, ... $ZrO_2$ 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.



Reference Number: 025003 NNORM

Rock Number: GS 15838

Chemical Analysis Locality: near Kuala Sungei Chemperdak, Pahang Name: DOLERITE

DATA CARD 1 Weight Percent

| | 1. $SiO_2$ | 2. $Al_2O_3$ | 3. $TiO_2$ | 4. $Fe_2O_3$ | 5. FeO | 6. MnO | 7. NiO | 8. MgO |
|---|---|---|---|---|---|---|---|---|
| Columns | 1 2 3 4 5 | 6 7 8 9 10 | 11 12 13 14 15 | 16 17 18 19 20 | 21 22 23 24 25 | 26 27 28 29 30 | 31 32 33 34 35 | 36 37 38 39 40 |
| | 046.53 | 014.88 | 002.18 | 002.93 | 010.10 | 000.11 | 000.00 | 006.97 |

| | 9. CaO | 10. BaO | 11. SrO | 12. $Na_2O$ | 13. $K_2O$ | 14. $P_2O_5$ | 15. $CO_2$ | 16. $ZrO_2$ |
|---|---|---|---|---|---|---|---|---|
| Columns | 41 42 43 44 45 | 46 47 48 49 50 | 51 52 53 54 55 | 56 57 58 59 60 | 61 62 63 64 65 | 66 67 68 69 70 | 71 72 73 74 75 | 76 77 78 79 80 |
| | 008.82 | 000.02 | 000.00 | 002.62 | 001.09 | 000.43 | 000.72 | 000.00 |

DATA CARD 2 Weight Percent

| | 17. F | 18. S | 19. $Cr_2O_3$ | 20. Cl | 21. $SnO_2$ | 22. $LiO_2$ | 23. CuO |
|---|---|---|---|---|---|---|---|
| Columns | 1 2 3 4 5 | 6 7 8 9 10 | 11 12 13 14 15 | 16 17 18 19 20 | 21 22 23 24 25 | 26 27 28 29 30 | 31 32 33 34 35 |
| | 000.00 | 000.05 | 000.02 | 000.10 | 000.00 | 000.00 | 000.00 |

| $H_2O+$ = 2.46 | $H_2O-$ = 0.32 | OTHERS: nil | Less O for OH,F,Cl,S 0.04 | TOTAL: 100.31 |
|---|---|---|---|---|

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 1. List of the normative minerals used in the programme.

| *Mineral* | *Abbreviation* | *Formula* |
|---|---|---|
| | | Salic Group |
| quartz | QTZ | $SiO_2$ |
| corundum | COR | $AlO_{1\frac{1}{2}}$ |
| zircon | ZIR | $ZrO_2$, $SiO_2$ |
| orthoclase | OR | $KO_{\frac{1}{2}}$, $AlO_{1\frac{1}{2}}$, $3SiO_2$ |
| albite | AB | $NaO_{\frac{1}{2}}$, $AlO_{1\frac{1}{2}}$, $3SiO_2$ |
| anorthite | AN | $CaO$, $2AlO_{1\frac{1}{2}}$, $2SiO_2$ |
| leucite | LC | $KO_{\frac{1}{2}}$, $AlO_{1\frac{1}{2}}$, $2SiO_2$ |
| nepheline | NE | $NaO_{\frac{1}{2}}$, $AlO_{1\frac{1}{2}}$, $SiO_2$ |
| kaliophilite | KP | $KO_{\frac{1}{2}}$, $AlO_{1\frac{1}{2}}$, $SiO_2$ |
| halite | HL | NaCl |
| plagioclase | PLAG | $AB+AN = AB_xAN_{100-x}$ |
| | | Femic Group |
| acmite | AC | $NaO_{\frac{1}{2}}$, $FeO_{1\frac{1}{2}}$, $2SiO_2$ |
| sodium metasilicate | NS | $2NaO_{\frac{1}{2}}$, $SiO_2$ |
| potassium metasilicate | KS | $2KO_{\frac{1}{2}}$, $SiO_2$ |

*(Table 1 continued)*

| *Mineral* | *Abbreviation* | *Formula* |
|---|---|---|
| wollastonite | WO | $CaO, SiO_2$ |
| enstatite | EN | $MgO, SiO_2$ |
| ferrosilite | FS | $FeO, SiO_2$ |
| forsterite | FO | $2MgO, SiO_2$ |
| fayalite | FA | $2FeO, SiO_2$ |
| calcium orthosilicate | CS | $2CaO, SiO_2$ |
| magnetite | MT | $FeO, 2FeO_{1\frac{1}{2}}$ |
| chromite | CM | $FeO, 2CrO_{1\frac{1}{2}}$ |
| hematite | HM | $FeO_{1\frac{1}{2}}$ |
| ilmenite | IL | $FeO, TiO_2$ |
| titanite | TN | $CaO, TiO_2, SiO_2$ |
| perovskite | PF | $CaO, TiO_2$ |
| rutile | RU | $TiO_2$ |
| apatite | AP | $9CaO, 6PO_{2\frac{1}{2}}, CaF_2$ |
| If there is no fluorine in the analysis, then AP = | | $5CaO, 3PO_{2\frac{1}{2}}$ |
| fluorite | FR | $CaF_2$ |
| pyrite | PR | $FeS_2$ |
| calcite | CC | $CaO, CO_2$ |
| cassiterite | CT | $SnO_2$ |
| diopside | DI | $WO_{50}EN_xFS_{50-x}$ |
| hypersthene | HY | $EN_xFS_{100-x}$ |
| olivine | OL | $FO_xFA_{100-x}$ |

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 $SnO_2$ 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 Sungei Chempedak, Pahang, Malaya (Alexander, 1964, pp. 38–39, specimen 02.5.003). In addition to the tabulated data, $H_2O+$ is 2.46 and $H_2O-$ is 0.32. NiO is recorded as 'trace' and SrO, $SnO_2$, $LiO_2$ 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 discrepencies in the results have alwasy been shown to result from the human element.

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      OXIDE    WEIGHT      CATION      GROUP CATION
               PER CENT    PER CENT    PER CENT

       SI       46.53       44.57       44.57
       AL       14.88       16.79       16.79
       TI        2.18        1.57        1.57
       FE3       2.93        2.11        2.11

       FE2      10.10        8.09)
       MN        0.11        0.08)       8.17
       NI        0.00        0.00)

       MG        6.97        9.95        9.95

       CA        8.82        9.05)
       BA        0.02        0.00)       9.05
       SR        0.00        0.00)

       NA        2.62        4.86        4.86
       K         1.09        1.33        1.33
       P         0.43        0.34        0.34
       C         0.72        0.94        0.94
       ZR        0.00        0.00        0.00
       F         0.00        0.00        0.00
       S         0.05        0.08        0.08
       CR        0.02        0.01        0.01
       CL        0.10        0.16        0.16
       SN        0.00        0.00        0.00
       LI        0.00        0.00
       CU        0.00        0.00
SALIC
        QTZ     COR     ZIR      OR      AB      AN      LC      NE      KP      HL              TOTAL
       0.000   0.000   0.000   6.659  23.517  26.908   0.000   0.000   0.000   0.324           57.409

FEMIC
         AC      NS      KS      WO      EN      FS      FO      FA      CS      MT      CM      HM      IL      TN
       0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000   3.167   0.022   0.000   3.140   0.000

         PF      RU      AP      FR      PR      CC      CT      DI      HY      OL              TOTAL
       0.000   0.000   0.929   0.000   0.134   1.883   0.000   8.619  18.982   5.709           42.590

DI =   8.619 WO(50)EN(32) FS(18)

HY =  18.982EN( 64)FS( 36)

OL =   5.709 FO( 64)FA( 36)

PLAG  50.425 AB( 47)AN( 53)

SALIC(57)FEMIC(43)

QTZ + OR + PLAG =  57.085   QTZ( 0)OR(12)PLAG(88)

  AN + AB + OR =  57.085     AN(47)AB(41)OR(12)

 QTZ + AB + OR =  30.176    QTZ( 0)AB(78)OR(22)
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Fig. 2. Actual example of the norm and cation-percentage computer output.

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 $P_2O_5$ to form apatite and with the $CO_2$ 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 re-calculated omitting either or both of $CO_2$ and $P_2O_5$ 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

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