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**DATAT - DATA1 - DATA2 - CORFL**

**A computer program for the off-line data reduction of thermionic mass spectra for isotopic analysis, recorded on paper tape by means of a Dataprint digital voltmeter**

by

**H.A. TASMAN**

**LIBRARY**

**1970**



**Joint Nuclear Research Center  
Karlsruhe Establishment - Germany  
European Transuranium Institute**

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DATAT - DATA1 - DATA2 - CORFL : A COMPUTER PROGRAM FOR THE OFF-LINE DATA REDUCTION OF THERMIONIC MASS SPECTRA FOR ISOTOPIC ANALYSIS, RECORDED ON PAPER TAPE BY MEANS OF A DATAPRINT DIGITAL VOLT-METER by H.A. TASMAN

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**DRFL**

**duction of thermionic  
on paper tape by  
meter**

**EUR 4476 e**

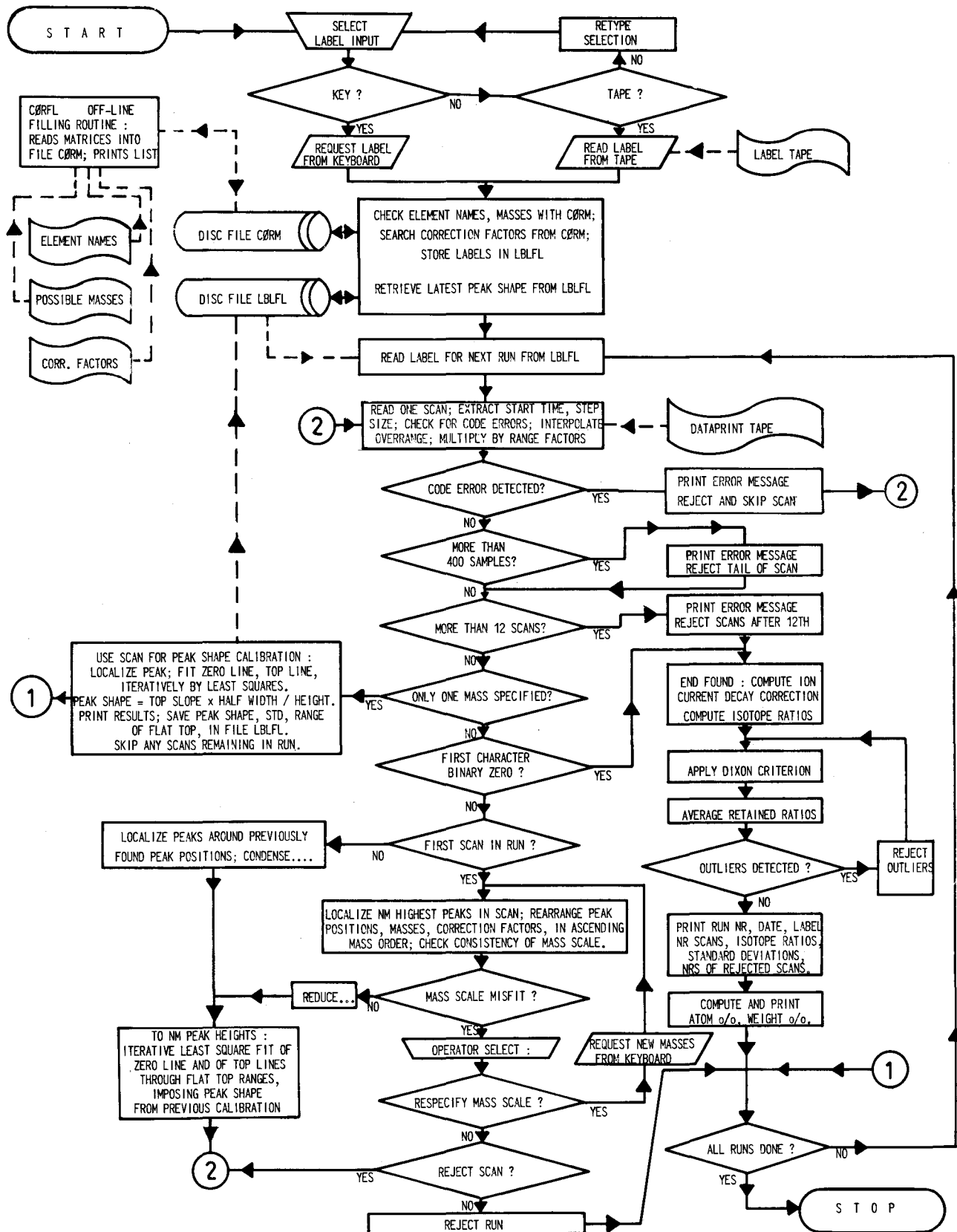
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**Abstract not available**

**KEYWORDS**

COMPUTERS  
PROGRAMMING  
THE MIONICS  
MASS SPECTROMETERS  
DIGITAL SYSTEMS  
ELECTRIC METERS



FLOW CHART OF COMPUTER PROGRAM FOR DATA REDUCTION OF ISOTOPE RATIO MASS SPECTRA, RECORDED ON DATAPRINT TAPE

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## 1. GENERAL \*)

### a. Purpose, program language

The increasing efficiency of routine mass spectrometer operation for thermionic isotopic analysis poses an ever increasing data reduction problem if analog recorded spectra are to be measured by hand. The time required for graphical interpolation of a slowly decaying mass spectrum, manual reading of the interpolated peak heights, and computation of the isotope ratios by hand by means of a programmed desk calculator, is of the same order as the time needs to record the spectrum.

As an intermediate solution, the "DATAPRINT" digital voltmeter with punched paper tape output (manufactured by Varian MAT Bremen) seems to offer interesting possibilities. The "DATAPRINT" integrates the input voltage by means of a voltage-to-frequency converter (full range corresponding to 50 kc/s output, 0.1% linearity) and a 16-bit binary counter, over a series of successive sampling intervals of preselected length, typically 160 ms. or 320 ms. Range switching is accomplished by amplification of the input signal. In the "DATAPRINT - Modell E" range selection is done by hand; the "DATAPRINT-Modell V" offers automatic ranging. Automatic reduction of the sensitivity on the rising edge of a peak is done after an over-range has been detected. Above its linear range, the V/F converter deviates so severely from linearity, that an overrange reading is essentially meaningless. The "DATAPRINT-Modell V" uses a common indicator for overrange and counter overflow, which is recorded on the paper tape output.

The present program was written to digest paper tape data in Dataprint code (see appendix 1) by means of the IBM-1130 digital computer. It is written in FORTRAN, except for the subroutines LEADR, LOAD, PTAPE and PGSFT which are written in ASSEMBLER language.

### b. Required equipment

The minimum requirements on the computer are 8K core memory, disc, paper tape reader and punch. Output is through the console typewriter and paper tape punch.

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\*) Manuscript received on 8 January 1970

c. Size

Together with the required monitor subroutines and library functions, the size of the program exceeds the capacity of the 8K-core storage. Execution is possible by separating the initializing part, (DATA1, DATAT) and using the LOCAL (Load-on-call) facility of the 1130 - Monitor for 10 subroutines. SOCALs (System overlays) can be avoided. The space requirements for the routines in LOCALs are equal to that for the largest one among them, as all LOCALs are loaded, when required, into the same area of memory. As a consequence, the program sometimes had to be cut up into portions of about the same size, without logical need to specify these as separate subroutines.

d. Execution times

The program comprises iterative fitting procedures. As a consequence, the computation time depends on the quality of the data, especially for long runs. As a rough guide the following figures can be given : (for 1130 with 3,6  $\mu$ s memory cycle)

- |  |                                     |
|--|-------------------------------------|
| 1) Loading the programs from the disc, initialization, print out of normal messages and end mark | 75 sec.                             |
| 2) If punched output is requested, add for paper tape leader and trailer                         | 15 sec.                             |
| 3) Peak shape calibration run, N samples   | (45 + N/6) sec.                     |
| 4) Isotope ratio run, short scans (N $\approx$ 75; NM=2, NS scans)                               | (70 + NS x 12.5) sec.               |
| 5) Isotope ratio runs, long scans (N $\approx$ 320; NM=3 - 9; NS scans)                          | (40 + NM x 10 + NS x (65+2.5 x NM)) |
| 6) Punched tape output   | approx. 20 <sup>sec.</sup> /run     |

The above figures include time for reading the input tape at 60 char./sec. and for print-out through the console typewriter at 16 char./sec., with correct page shift, but without intermediate results. If error conditions occur, time for printing the error message and for corrective action has to be added, the latter being notable only if operator selection is required or if input data are to be skipped.



e. Definitions

Throughout the following pages, a number of terms are used that deserve a further definition:

Of each sample to be analyzed, a number (1 to 12) of consecutive scans is recorded to allow interpolation for ion current decay. This series of scans is called an analysis or run, and is separated on the DATAPRINT tape by binary zeros from the next run. Up to 53 runs may be recorded on one tape. From one sample, more than one run may be recorded, each of which is treated independently.

Each scan is recorded in the form of a series of integrated readings over consecutive sampling intervals, which are called sample readings or samples.

An indication of the quality of the data is obtained through the standard deviation of a variable  $x$ , defined as  $\sqrt{(\sum_1 (x_1 - \bar{x})^2)/(n - 1)}$ . This represents the standard deviation in the individual reading, and assumes a Gaussian distribution (which holds only for deviations that are small compared to the value in question). These standard deviations are listed alongside a value that represents the mean of the results for the variable in question. The reason for not stating the standard deviation of the mean instead, lies in the fact that statistical variations present only one contribution to the total uncertainty and the standard deviation of the mean suggests a better quality that is justified. The standard deviation as printed serves only as an indication of the quality of the data, and is independent of the number of scans.

## 2. FORMAT OF THE DATAPRINT-RECORDED MASS SPECTRA.

The Dataprint tape should be preceded by a leader, and ended with a trailer, of blanks (binary zeros).

The program requires at least once a single (slow) scan of one large peak for peak shape calibration. The peak shape is extracted and stored on the disc. Additional peak shape calibrations may be inserted anywhere in a series of runs, but should be specified accordingly (see 3.). If a run, specified as a peak shape calibration, contains more than one scan, a warning is printed, and the rest of the run is rejected. Computation is always done using the last peak shape calibration.

The isotope ratio mass spectra should be in the form of from 2 to 12 immediately succeeding scans. Scans after the 12th are rejected with print-out of a warning.

Each run should be followed by at least 5 blanks (binary zeros). Each scan should not contain more than 400 samples. If it does, an error message is printed and the tail after the 400th sample is rejected.

In one job a series of up to 53 runs or analyses can be specified. Preferably, the corresponding dataprint data should be on one tape, binary zeros separating runs, such as to allow continuous computation without operator intervention. Tapes from individual runs may be spliced together

For negative peaks dataswitch 8 should be up, for positive peaks it should be down. Internally the program operates on peaks of negative sign; if dataswitch 8 is down, the sign of the sample readings is inverted in the loading routine, and a sample readings print - out shows the inverted sign.

For correct fitting of the zero line between peaks, the zero should be adjusted to be identical to the electrical zero with a tolerance of  $\pm 1\%$  of the largest peak in the scan. The spectras should be recorded at such a resolution that the width of the zero between peaks equals at least that of the peak plateau.

### 3. SPECIFICATION OF THE RUNS IN A JOB (LABEL)

In one job from 1 to 53 runs or analyses may be specified. This label input may be either from the keyboard or from paper tape. For DATA1 the tape should be in PTTC/8 code; DATAT is identical to DATA1 except that it accepts ASCII-code tape. The format is identical for both inputs and indicated in appendix 3. The input medium is selected by typing 'KEY' or 'TAPE' when so requested by the program. When the input is through the keyboard, the data requested and the required format are specified for each entry.

The label consists of :

- a. Number of runs, and date.
- b. For each run: Analysis number and 'tag', element name, number of masses, masses. The 'tag' accepts two alphameric characters, and may be used for additional specification. The first mass entered serves as reference mass for isotope ratio calculation, the other masses may be entered in any order. Up to 10 masses may be specified. If one mass only is specified, the first scan of the run is taken as a peak shape calibration on the largest peak it contains. If more scans follow, they are rejected and a warning is printed.

4. CHECK ON THE LABEL ENTRIES. DATA1-DATAT

The program checks whether the number of runs is between 1 and 53, and whether the number of masses is between 1 and 10. Exceeding these limits causes an error message to be printed. When the input is from the keyboard, the same entry is requested again; if the input is from tape, a STOP/CALL EXIT follows

The label data are compared with a correction matrix CORM stored on the disc. This matrix is loaded off-line by a separate routine CORFL (see 7). It contains 10 element names, and for each element, up to 10 masses and the corresponding correction factors for mass discrimination.

If the element name does not match with one entry in CORM, the warning 'INCORRECT ELEMENT NAME' is printed, and the correction factors are put equal to unity. If any mass entry does not match with a mass specified for the element in question, the warning 'MASS NOT IN CORRECTION MATRIX' is printed, and the correction factor is put equal to unity.

The element name, the tags, and the date are read in A-format, and reproduced as entered on the print-out. If the entries for the number of runs or the number of masses are no integers (i. e. if they contain a decimal point, or other non-numeric characters than a blank), the machine stops at \$PRET (= adress/0028); pressing 'PROGRAM START' causes an error message to be printed as when exceeding the limits on these variables, followed by a 'STOP/CALL EXIT' or a new request for the entry in question.

A non-integer analysis number or mass results in the same stop at \$PRET. Restart with an incorrect analysis number results in a normal computation, except that the faulty number is reproduced as an integer in I4-format in the output; when the integer equivalent exceeds the capacity of the I4-field, \*\*\*\* is printed. Restart with a faulty mass causes a mass scale misfit to be signaled (see 11.), provided that more than 2 masses were specified; otherwise the incorrect masses are reproduced in the output.

The labels of all runs are stored on the disc in the file LBLFL, and retrieved one by one for each run as necessary.

## 5. OUTPUT OPTIONS

On execution of the program DATA1 or DATAT the machine prints a listing of the output options provided by the program. It is possible to specify correct page lay-out, print-out of individual sample readings, peak positions, peak heights, peak heights corrected for ion current decay, individual isotope ratios, by raising dataswitch 14, 13, 11, 12, 10, and 9 respectively. Raising dataswitch 0 causes a leader of binary zeros and delete codes to be punched; except for peak shape calibration runs, analysis nr. and tag, masses, and isotope ratios are punched on paper tape, for later use in isotope dilution calculations. Raising dataswitch 4 causes rejection of a run in case of mass scale misfit, without operator intervention (see 11.)

If switch 14 is down, the print-out of the results of each run is preceded by 8 blank lines; if it is up, the results of each run are printed on a new page, referring to the perforations every 72 lines of the console printer paper. Because the 1131 typewriter does not have a form-eject or page shift contact, the lines are counted as they are printed, and an initial adjustment of the perforation to the guide rail edge is necessary; manual line feeds disturb the lay-out and should be avoided after the initial synchronization.

The print-out of sample readings, peak positions, and peak heights is only intended for exceptional checking. The individual isotope ratios should be more generally useful for detection of contamination with a different element through a monotonous shift in the isotope ratio in the course of a run.

## 6. REMARK ON THE MASS SPECIFICATION

If NM masses are specified, the NM highest peaks are searched, and their positions are compared with the mass scale to check for misfit. This implies that the first scan of a run should not contain uninteresting peaks that are higher than the smallest peak of interest, or that all such peaks should be specified. To allow correct isotope

percentages for long irradiated uranium, that may contain more Np-237 than U-234, a special routine is included which eliminates the mass 237 before computing percentages if the element name is specified as 'U' or 'U'; the 237-peak is included in the isotope ratios, however.

#### 7. ROUTINE CORFL FOR FILLING OR CHECKING THE CORRECTION MATRIX CORM.

This routine accepts paper tape data to fill the element matrix, Format(10(1X,A2)) the mass matrix, Format (10 I 7), the correction factor matrix Format (10 F 7.4). The i-th element name corresponds to the i-th mass record and the i-th correction factor record. The order of masses is arbitrary, the corresponding correction factors should be introduced in the same order. If less than 10 masses are specified, dummy entries of arbitrary integer value should be introduced in the unused mass positions, dummy reals in the unused correction factor positions.

Loading of any of the three matrices may be skipped, so that only the correction factors or masses may be changed without changing the rest. Finally, a listing of the contents of CORM is printed for checking purposes; if all loading is skipped, this allows a check of the current content.

## 8. GENERAL FLOW DATA 2

At the conclusion of the initializing routine DATA 1 or DATA T, a link is made to the main program DATA 2 that controls the actual computation.

One scan is read (subroutine LOAD) and digested before the next scan is read. If one mass is specified, the first scan of a run is taken as peak shape calibration (subroutines PEAKS). If more than one mass is specified, successive scans are reduced to peak heights through the subroutines FIRST, CONDS, PKTOP, and, after the end mark is read (binary zeros), the peak heights are corrected for ion current decay by a linear interpolation to the start of the scan, using the preceding scan, and isotope ratios to the reference peak are calculated (subroutine COMPT). On these ratios, the DIXON outlier criterion is applied, outliers are rejected. The means of the retained ratios are computed and printed with their standard deviations and the numbers of rejected scans. Atom percents are computed and printed, together with standard deviations, computed through the propagation of errors (subroutine PRTPC). Finally, weight percents are computed and printed. After the last run has been digested, an end mark is printed, and a trailer of delete codes followed by binary zeros is punched if paper tape output had been requested (link to main program ENDMK).

## DETAILED PROGRAM DESCRIPTION

### 9. LOAD, Loading routine

The loading and conversion routine LOAD performs the following operations:

If the scan is the first of a run, the leader is skipped until a time mark is found. If it is not the first scan, the first character is retrieved from memory. The starting time and the step size are extracted. Consequently, the successive sample readings are read and converted, until a new time mark or a binary zero (end mark) is encountered, which is saved in memory. The time-step characters and the first character of each sample triad is checked for code errors. If a code error is detected, an error message is printed, indicating the position of the erroneous character, and rest of the run is skipped; compilation of this run is suppressed. If more than 400 samples are found in a scan, only the first 400 are converted. If an overflow or overrange is detected, the reading is considered as meaningless, and replaced by an extrapolation from the two previous readings. If the next reading is not overflow or overrange, the extrapolated value is replaced by the mean of the adjacent readings.

The time counter counts modulo  $2^{10}$ . The time reading of the first scan is accepted as such. For successive scans, the current time reading is increased by 0, 1024, 2048, etc. until the sum of the previous time reading and the present scan duration is less than the current reading. This assumes the number of samples in successive scans to be approximately the same, or more precisely: the difference in scan duration should not exceed the dead time between scans.



#### 10. PEAKS, Peak Shape Extraction Routine.

The peak shape is extracted by PEAKS through the following steps:

The highest (i. e. most negative) point is searched (subroutine SRXTR), subroutine LOC finds the points at half maximum at both sides of the top, subroutine LOCLZ fixes the peak position as the mean of the half-maximum points, and checks whether the half-width is less than 3 channels. If so, the peak is considered as a spike, eliminated, and the above procedure is repeated. If the half-maximum points cannot be found within the range scanned (because the peak lies at the boundary of the scan, and may be a spike) the error message 'ERROR IN LOC INPUT DATA' is printed, and the run is rejected.

Then a zero line is fitted by least squares through all points except those in the range of the peak top  $\pm 1.5 \times$  half-width, iteratively, rejecting those points that differ more than  $1x$  standard deviation from the last iteration. Similarly, a straight line is fitted iteratively through the peak top. The peak shape, defined as the slope times the half-width divided by the height, is recorded on the disc, together with the standard deviation of the top line, and the range of the flat top, expressed in half-width units. The latter is defined as the range beyond which two successive points deviate more than one standard deviation from the line fitted through the peak top.

The results are printed, but not punched on tape

11. FIRST, routine for digesting the first scan of an isotope ratio run.

If the number of masses requested (NM) is greater than unity, the routine FIRST localizes the NM highest peaks by means of the routines LOCLZ, SRXTR, LOC, described under 10. Scanning of the range of  $\pm 1.5 \times HW$  around previously found peak positions is suppressed through the function IELIM, where HW represents the half-width of the first (= highest) peak found in the current scan. In case of 'ERROR IN LOC INPUT DATA' (see 10), the scan is rejected.

Subsequently, the peak positions and the specified masses are re-arranged in ascending order. The scale factor (= the number of channels per mass unit) is computed for each pair of successive values. The minimum and the maximum value of the scale factor is searched. If the difference between the maximum and the minimum exceeds the half-width of the largest peak, the error message 'MASS SCALE MISFIT' is printed, followed by the positions of the NM highest peaks and the masses that were specified. If dataswitch 4 is up, the run is then rejected without operator intervention; if dataswitch 4 is down, the operator may select either rejection of the current scan, respecification of the mass scale, or rejection of the run, by typing '2', '3', or '4' respectively. If '2' is typed, the next scan is read and treated as if it were the first one. If '3' is typed, the machine requests keyboard entry of the number of masses NM, and of the masses. All keyboard entries are checked:

If another digit than 2, 3, or 4 is entered, the machine answers 'RETYPE OPERATOR SELECTION' and requests a new entry. If a non-numeric character is typed, the machine stops a ~~S~~PRET with /F003 in the accumulator; restart causes the same retype request to be printed. The number of masses is checked to be within the range 2 to 10 and at least equal to the original entry; if outside this range, a warning is printed and the request is repeated.

If the entry for NM is not an integer (contains another non-numeric character than a blank) a stop at ~~SPRET~~ occurs as above, restart results in a new request for the entry.

The mass value entries are checked only whether integer; if not, a stop at ~~SPRET~~ occurs which can be restarted.

After respecification of the mass scale, the correction factors are assumed to be unity. A new check for mass scale misfit is made, with the same facilities for operator selection as above.

It should be remarked, that the mass scale check is only possible if more than 2 masses are specified. If so, this check virtually eliminates faulty mass entries (or mass entries outside the correct format), and allows these errors to be corrected at computation time.

## 12. PKTOP Routine for reducing a scan to peak heights

Once peak positions are established, a line is fitted through all points except the peak top ranges, iteratively by least squares, and a zero correction is applied. Then a line is fitted through the flat top range of each peak, using the half-width of the largest peak in the first scan of the present run and the slope-to-height-ratio imposed by the latest peak shape calibration. The least square fit through the peak top is done iteratively, using only points within the flat top range that deviate less than twice the standard deviation from the last line computed. The peak height is taken as the height of the top line at the peak position.

### 13. CONDS Routine for localizing peaks in successive scans

In the scans after the first one, the peaks are localized in the range around the found peak positions. This is done to assure that reference is always made to the same peaks even if a contamination might 'grow in' in the course of a run. At first, localisation is attempted between the 'foot-points' of the peak; the edges are assumed to be S-shaped, centro-symmetric around the half-maximum point, up to the limit of the plateau. Whereas this procedure operates correctly for spectra recorded at a resolution at least twice as high as the mass in question, in lower resolution spectra a small peak adjacent to a large one may be missed, as the search locks in on the tail of the large neighbour. This causes two successive peak positions to be identical. Then scanning range is reduced to  $\pm HW/2$  around each previous position, and the search is repeated. After localization, each scan is reduced to peak heights through PKTOP.

#### 14. COMPT - DIXON - PRTPC Routines for final data reduction.

From the second scan onward, the peak heights are corrected for ion current decay by a linear interpolation to the start of each scan, using the peak heights from the previous scan, and the time information read from the Dataprint tape by the LOAD routine. If dataswitch 10 is up, the decay-corrected peak heights are printed.

If only one scan is present (only one scan enregistered), or all scans except the last rejected through operator intervention after mass scale misfit, the peak heights are taken such.

The corrected peak heights are then divided by the reference peak height, and the 'mass discrimination' correction factors are applied. If dataswitch 9 is up, the individual isotope ratios are printed, as well as the applied correction factors.

The isotope ratios for each mass are then re-arranged in ascending order. The DIXON outlier criterion ('Experimental Statistics', Ch. 17, NBS Handbook 91 (1967)) (95% confidence) is applied on the highest and the lowest value of each ratio. If an outlier is detected, the ratio is rejected and the procedure repeated. The means of the retained ratios are computed, as well as the standard deviations  $(\sigma_i = (\sum A_i^2 / (n-1))^{1/2})$ .

The isotope ratios are printed, with the standard deviations and the numbers of the rejected scans, if any, a zero indicating that none were rejected. If dataswitch 0 is up, analysis nr, tag, number of masses, masses and isotope ratios are punched in paper tape. The isotope ratios are then converted to atom percentages. The corresponding standard deviations are obtained from the relation:

$$\sigma_{pi} = \sqrt{\sum_{j=1}^{NM} \left\{ \left( \frac{\partial PI}{\partial J} \right)^2 \sigma_j^2 \right\}}$$

where: J stands for the isotope ratio of mass j

PI is the percentage of mass i;

$\sigma_j$  and  $\sigma_{pi}$  are the corresponding standard deviations

The atom percentages and their standard deviations are printed.

Finally, the data are converted to weight percentages, which are printed.

15. ENDMK - Normal Exit

After all runs have been done, the message 'ALL RUNS DONE, JOB TERMINATED CORRECTLY' is printed, and if paper tape output had been requested, a trailer of delete codes followed by binary zeros is punched.

16. ERRM2, ERRM3, ERRM4 Error messages

The error message for code error, too long scans or more than 12 scans, are contained in short separate subroutines, which are loaded as LOCAL only in the exceptional case of error condition. Error messages are printed in red.

17. OPERATING INSTRUCTIONS DATA 1 -(DATAT), DATA2

The identification data should preferably be prepared in advance on paper tape through the routines called by `//6 XEQ6 PTUTL` or `//6 XEQ6 W`, according to the format in appendix 3. Up to 53 runs may be specified for one job, on all of which the same date will be printed. For a few runs only, the identification may be entered through the keyboard at DATA 1 execution time.

The program is called by the record `//6 XEQ6 DATA 1`, <sup>or `// XEQ DATAT`</sup> entered either from tape or (after `//6 TYP`) from keyboard. If a system error caused the preceding job to be aborted, the above call should be preceded by `//6 JOB`.

On execution of DATA 1 a message is printed which lists the available output options (see 5.). Of these, paper tape output (switch 0 up) and correct page lay-out (switch 14 up) should be selected before restart. If these are selected during execution of a job, the page lay-out may be incorrect, and/or the paper tape leader may be missing. These options may be suppressed during execution, in which case a paper tape trailer may have to be punched manually. The other output options may be switched on or off as desired during execution, so that only intermediate results of selected parts can be printed through operator selection, without otherwise disturbing compilation. If any of the switches 9 - 13 have been up during the compilation of one run, at least one of them should be left up immediately prior to the print-out of the final result, as this triggers a shift to a new page. During the print-out of the final results of a run, any of the options 9 - 13 may be switched off for the next run.

After restart, the machine requests selection of the identification input; 'KEY' or 'TAPE' should be typed when so requested. In the former case, the entries are specified as required by the machine, together with the format. In the latter case, the identification tape should be in the reader and the reader should be readied. If the reader is not ready, the machine stops at `#PRET` and can be restarted by pressing 'PROGRAM START' after readying the reader.

If the identification tape contains intolerable errors (number of runs outside the range 1 - 53, number of masses outside the range 1 - 10), an error message is printed and a STOP/CALL EXIT results. In this case a corrected tape should be prepared and the program be called anew. Non-integer entries for analysis numbers or masses cause a stop at `#PRET` with `/F009` in the accumulator; restart causes resumption of computation with the erroneous entries. If the masses are in error and more than 2 masses were specified, a mass scale misfit is usually signalled during computation (see 11), which allows for correction. Of course, the execution of any program may be stopped at any moment if an error is detected, and executed from the start by a cold start followed by a new call.

When the identification for all runs has been entered, the program requests loading of the Dataprint tape and stops; it should be restarted after the leader of this tape is put in the reader. Preferably, all data from all runs should be on one continuous tape, at least three binary zeros separating runs; tapes from successive runs may be spliced together.

After pressing 'PROGRAM START', the scans are read one by one and digested. The reader head should not be raised when the reader has stopped at a start of a new scan, as a reading error will result. After a stop at the end of a run, on a binary zero, raising the head is allowed. This makes it possible to load the tape of the next run (leader in the reader) after the last scan of the previous run has been read. This procedure is not recommended, however, as it requires continuous operator attention for uninterrupted computation.

When a code error is detected, the run is rejected, and a message is printed, indicating where the error was found. A code error may be caused by a 1132 reader error, or an erroneous character may be present on the Dataprint tape. In this case, the tape of the erroneous run should be selected and rerun; if the same code error is detected again, the tape



is probably in error, and can be inspected visually. Reader errors can also be caused by exceeding the mechanical tolerances on the punching of the holes, especially in the spacing of the characters.

If unattended operation is required, Dataswitch 4 should be raised to reject a run with mass scale misfit without operator intervention. Apart from the stops after erroneous entries in case of mass scale misfit, indicated in 11, any stops before the correct end of the job are either due to the reader or punch going not ready (tape in the reader damaged, or lever on the punch raised) - or to a machine malfunction. Of these stops, only the punch-caused stop can be restarted without error; in the other cases, the Dataprint tape of the correctly treated runs should be separated, a new job prepared, and the remaining tape run after a fresh call of DATA1 or DATAT. It is possible to repeat the computation of all runs without entering the identification label anew, by placing the start of the Dataprint tape in the reader, and executing DATA 2 (//6 XEQ6 DATA 2); the page lay-out, however, will then be incorrect.

18. ERROR STOPS AND REMEDIES.

To assist identification, all error messages and warnings are printed in red.

a. If an error was detected in the label tape, or if the label tape was not accepted by the program, make a listing with PTUTL, copy the correct parts and add, delete or change as required. To list a tape, raise switches 0 and 1, to copy, raise 0, 1, and 3; switch 15 causes a stop after reading.

b. If a 'CODE ERROR' is detected, locate the defective run, place it in the reader, call DATA 1 or DATAT from the keyboard, enter the label for the defective run through the keyboard, and try again. If the same code error is detected again, inspect the dataprint tape at the indicated position. During the print-out of the code error message, the reader has stopped one character after the defective one.

c. MORE THAN 12 SCANS IN RUN' do not require operator intervention, the scans after the 12th being skipped by the program.

d. MORE THAN 400 SAMPLES IN SCAN' do not require operator intervention, the tail of the scan being skipped by the program. However, it is to be verified whether any essential information is lost; occasionally a mass scale misfit may be signaled.

e. The mention 'ERROR IN LOC INPUT DATA' indicates, that a peak is found at the beginning or at the end of a scan, and causes the scan to be skipped. The mass spectrum should be rerun with a scanning range set such that the scans are neither started nor stopped on a peak higher than the smallest peak of interest.

f. An attempt to enter a character illegal in the specified format, causes the machine to stop at ~~S~~PRET. It can be restarted by pressing 'PROGRAM START'. If the entry was through the keyboard, the program may repeat the request. If not, the faulty entry will appear on the print-out; in case of faulty masses, the weight 0/0 will be in error.

#### 19. OPERATING INSTRUCTIONS FOR CORFL.

Prepare a tape containing any of the following three:

- a. Element names - Format ( 10 (1X, A2) )
- b. Masses - Format ( 10 I 7 )
- c. Correction factors - Format ( 10 F 7.4 )

Call CORFL ( // XEQ CORFL)

Place the tape, if any, in the reader.

Type '1' to load the desired matrix, type '2' to skip loading, as requested by the program.

Finally, a listing will be printed of the contents of CORM.

APPENDIX 1

D A T A P R I N T C O D E

/	must be no hole	
O	must be hole	
.	sprocket hole	If information is
T	time bit	distributed over more
S	step bit	than one character, the
*	sample bit	most significant bits
\$	sample sign	are
R	range bit	contained in the first
#	overflow, overrange	character. the least signifi
		in the last character

S B A C 8 . 4 2 1	Track
-----	
// // // // . // // //	Leader of binary zeros
// // // // . // // //	Minimum length 12
// // // // . // // //	characters
-----	
O O / T T . T T T	First Time/ Step Triad
O O / T T . T T T	Time in 0.1 s. units
O / O / / . S S S	Sample time = 20 <sup>step</sup> ms.
-----	
O O O * * . * * *	
# R R * * . * * *	First Sample Triad
# R \$ * * . * * *	
-----	
O O O * * . * * *	
# R R * * . * * *	Second Sample Triad
# R \$ * * . * * *	
-----	
O O O * * . * * *	
# R R * * . * * *	Last Sample Triad of
# R \$ * * . * * *	First Scan
-----	
O O / T T . T T T	
O O / T T . T T T	Time/Step Triad of Next Scan
O / O / / . S S S	
-----	
O O O * * . * * *	
# R R * * . * * *	First Sample Triad of Next Scan
# R \$ * * . * * *	
-----	
O O O * * . * * *	
# R R * * . * * *	Last Sample Triad of Last Scan
# R \$ * * . * * *	
-----	
// // // // . // // //	Trailer of Binary Zeros
// // // // . // // //	Minimum length : 5 characters if
// // // // . // // //	more runs follow on same tape;
// // // // . // // //	12 characters at end of tape

# APPENDIX 2 PTTC/B PAPER TAPE CODE

CASE	S	B	A	C	B	.	4	2	1	TRACK	CASE	S	B	A	C	B	.	4	2	1	TRACK	
U	●	●							●	A	L			●	●					●	0	
U	●	●							●	B	L									●	1	
U	●	●	●						●	C	L			●	●					●	2	
U	●	●	●	●					●	D	L			●	●					●	3	
U	●	●	●	●					●	E	L			●	●					●	4	
U	●	●	●	●					●	F	L			●	●					●	5	
U	●	●	●	●					●	G	L			●	●					●	6	
U	●	●	●	●					●	H	L			●	●					●	7	
U	●	●	●	●					●	I	L			●	●					●	8	
U	●	●	●	●					●	J	L			●	●					●	9	
U	●	●	●	●					●	K	L	●	●	●	●					●	.	
U	●	●	●	●					●	L	L	●	●	●	●					●	( +	
U	●	●	●	●					●	M	L	●	●	●	●					●	&	
U	●	●	●	●					●	N	L	●	●	●	●					●	\$	
U	●	●	●	●					●	O	L	●	●	●	●					●	*	
U	●	●	●	●					●	P	L	●	●	●	●					●	)	
U	●	●	●	●					●	Q	L	●	●	●	●					●	/	
U	●	●	●	●					●	R	L	●	●	●	●					●	↓	
U	●	●	●	●					●	S	L	●	●	●	●					●	↑	
U	●	●	●	●					●	T	L	●	●	●	●					●	=	
U	●	●	●	●					●	U	L	●	●	●	●					●	#	
U	●	●	●	●					●	V	L	●	●	●	●					●	&Agrave;	
U	●	●	●	●					●	W	L	●	●	●	●					●	&Ograve;	
U	●	●	●	●					●	X	L	●	●	●	●					●		
U	●	●	●	●					●	Y	L	●	●	●	●					●		
U	●	●	●	●					●	Z	L	●	●	●	●					●		
U	●	●	●	●					●	TAB	L	●	●	●	●					●		
U/L	●	●	●	●					●	LC	L	●	●	●	●					●		
U/L	●	●	●	●					●	LOWER CASE	L	●	●	●	●					●		
U/L	●	●	●	●					●	DEL	L	●	●	●	●					●		
U/L	●	●	●	●					●	DELETE	L	●	●	●	●					●		
U/L	●	●	●	●					●	RES	L	●	●	●	●					●		
U/L	●	●	●	●					●	RESTORE	L	●	●	●	●					●		
U/L	●	●	●	●					●	NL	L	●	●	●	●					●		
U/L	●	●	●	●					●	NEW LINE	L	●	●	●	●					●		
U/L	●	●	●	●					●	BS	L	●	●	●	●					●		
U/L	●	●	●	●					●	BACKSPACE	L	●	●	●	●					●		
U/L	●	●	●	●					●	LF	L	●	●	●	●					●		
U/L	●	●	●	●					●	LINE FEED	L	●	●	●	●					●		
U/L	●	●	●	●					●	EOB	L	●	●	●	●					●		
U/L	●	●	●	●					●	END OF BLOCK	L	●	●	●	●					●		
U/L	●	●	●	●					●	RS	L	●	●	●	●					●		
U/L	●	●	●	●					●	READER STOP	L	●	●	●	●					●		
U/L	●	●	●	●					●	UC	L	●	●	●	●					●		
U/L	●	●	●	●					●	UPPER CASE	L	●	●	●	●					●		

(ü)

(Ä)  
(Ö)

(log. OR)  
(log. NOT)

# DATENKARTEN

Programm DATA1 - LABEL Datum 29.09.69 Name H. A. TASMAN Blatt-Nr. 1

NR	DATE	NUMBER OF RUNS, DATE FORMAT (I2, 1X, 5A2)												
ANAL. NR	TAG	EL	NM	ANALYSIS NR., TAG, ELEMENT NAME, NUMBER OF MASSES FORMAT (I4, A2, 1X, A2, 1X, I2)										
REF. MASS	MASS(j)	MASS(j)	....	....	....	....	....	....	....	MASS(n)	MASSES (REFERENCE = FIRST ENTRY) FORMAT (10I4) (FILL AS FAR AS REQUIRED)			
ANAL. NR.	TAG	EL	NM	} SECOND RUN										
REF. MASS	MASS(j)	MASS(j)	...											...
.														
.														
ANAL. NR.	TAG	EL	NM	} LAST RUN										
REF. MASS	MASS(j)	MASS(j)	...											...

APPENDIX 3

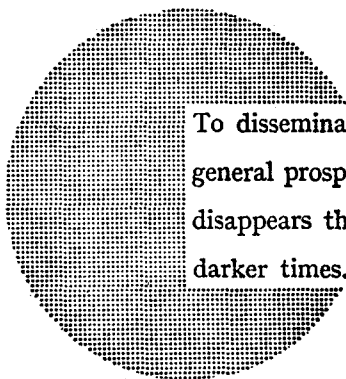
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To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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