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Professional paper

A POSSIBLE SOLUTION TO LabCalc PROBLEMS

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Among many outstanding features for spectra manipulation (*FLAT, SMOOTH, CURVEFIT* etc.), as well as a number of import-export data-file drivers, the LabCalc programming package appears to suffer from a trivial, yet annoying shortcoming: the input stream of data have to be organized as a set of equidistant points. As a result, a number of ASCII data files are useless in their original form. The problem may be overcome by interpolation. A simple QBASIC program was written, to transfer the spectra files from their original to a form recognizable by the LabCalc package.

Key words: file transfer, data interpolation, spectra

Research workers at both the Institute of Chemistry (Faculty of Natural Sciences and Mathematics) and the Institute of Technology (Faculty of Technology and Metallurgy), as well as those working at research centers (e.g. OHIS) widely use the programming package for spectra manipulation, known as LabCalc[1].This almost superb program (which operates under MS-DOS) has quite a number of outstanding features: difference spectra, first and higher derivatives, integration, flattening, smoothing, deconvolving and many other useful operations are performed within few key-strokes. IR, UV, Raman and NMR spectra, chromatograms, DTA curves *etc*. may easily be manipulated. Also, the program has a number of drivers that convert original data into standard LabCalc spectra file form (.SPC). It seemed that everything works perfectly, until we came across spectra files, the data of which were acquired from a DILOR Raman spectrometer.

The files are of ASCII type and could be edited by the standard DOS 5.0 editor. Basically, they are X-Y data pairs with a header and are preceeded with some additional information. The first line of the files reads "Version 2.00". Two import/export DILOR drivers were found in the LabCalc package, the one denoted as DILOR_2 being designed for version 2.00 format of the spectra. This driver was used; the spectra were imported without problems and converted to .SPC format. The Raman spectrum of one of these compounds (probably $KH_2PO_2 \cdot H_3PO_2$) is shown in Fig. 1. Everything seemed to be normal, except that the P-H stretching bands were unusually low, much lower than the corresponding bands in the IR spectrum.

Fortunately, the operator handed us a plot of the acquired data. This Raman spectrum is presented in Fig. 2.

Apart from the great similarity of the spectra, it is clear that the bands in the latter spectrum are shifted with respect to the bands in the first one. This spectrum is in much closer agreement with the IR spectrum of the compound.

Initially, we assumed that the driver might not be the right one. We changed the driver from a DILOR_2 to an ASCII_XY and deleted the redundant lines in the original file (the one containing acquired data). Upon importing and converting, the spectrum matched exactly the one presented in Fig. 1. Obviously, the problem was intrinsic to LabCalc.

A closer inspection of the acquired data file revealed that the data spacing (the X-coordinate) slightly increases when moving through the file from the first to the last data point. Could this, perhaps, cause the trouble? In order to check this, we exported the converted LabCalc file (.SPC) into the original (DILOR) format and to our surprise a stream of equidistant points was generated! For some unknown reason, LabCalc was designed to deal only with equally spaced points as a legal input; this is slightly inconvenient. However, LabCalc does not alert the user that the input format is unacceptable! And this is really very inconvenient, not to say more. Using LabCalc in such cases may become hazardous.

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1 Galactic Industries Corporation, 395 Main, Salem, NH 03079, U.S.A

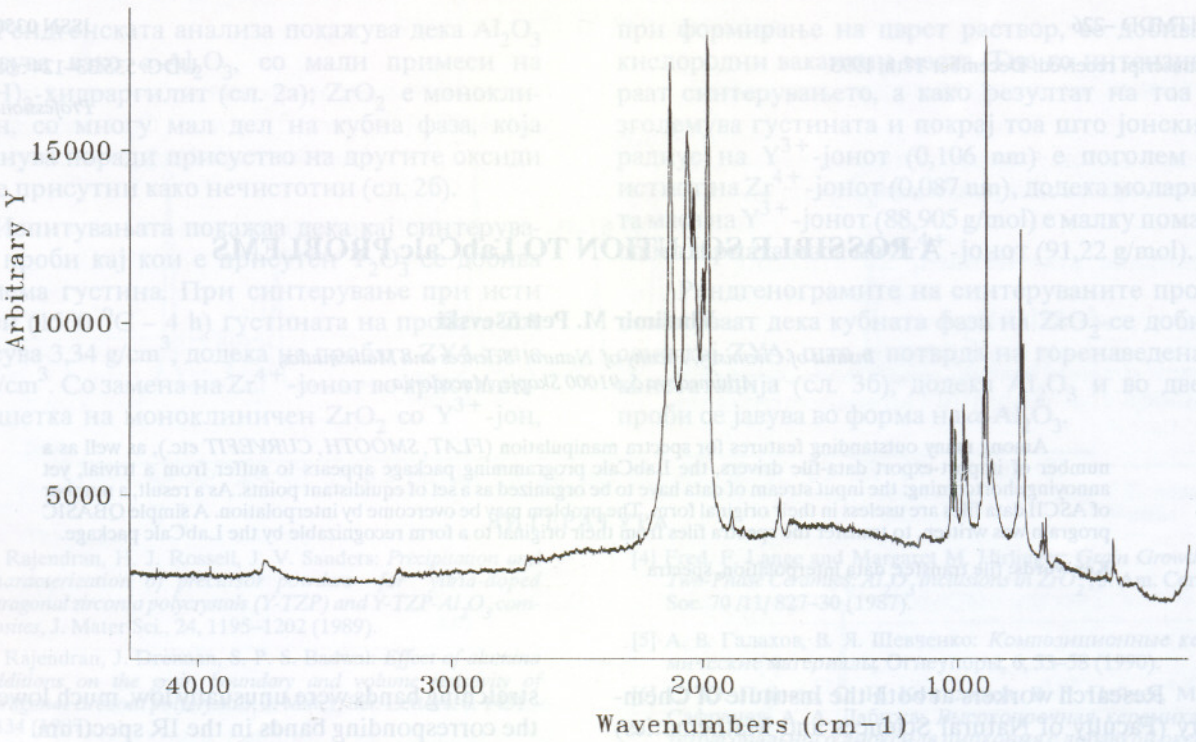

Fig. 1. Raman spectrum of $KH_2PO_2 \cdot H_3PO_2$ – LabCalc plot of the imported file using DILOR_2 driver

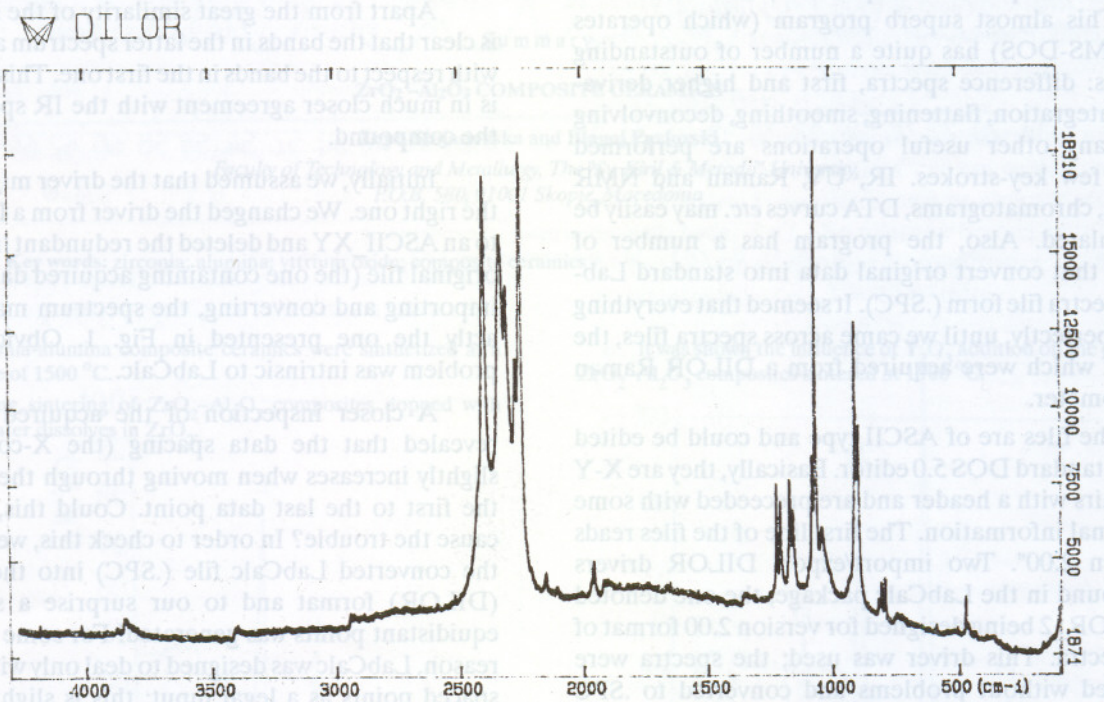

Fig. 2. Raman spectrum of $KH_2PO_2 \cdot H_3PO_2$ – LabCalc plot of the acquired data

In order to solve the problem, we generated an equidistant set of data points. A simple linear interpolation was used for that matter, as the original data points were close enough. A BASIC coded program was written (see the Appendix for details). After the original data points were converted to an equidistant set, this (intermediate) file was imported to LabCalc with the ASCII_XY driver. The final spectrum is presented in Fig. 3.

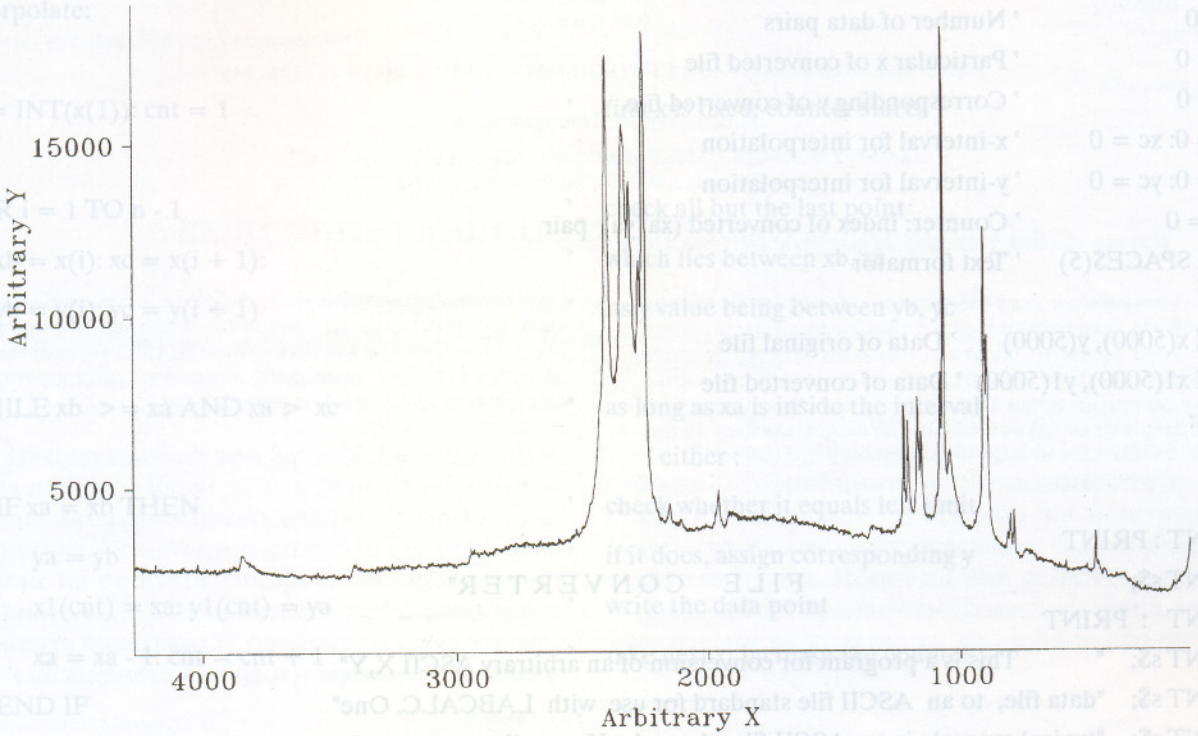

Fig. 3. Raman spectrum of $KH_2PO_2 \cdot H_3PO_2$ – LabCalc plot of the imported intermediate file (generated by interpolation from the acquired data) using ASCII_XY driver

As seen, the spectrum is for all practical purposes identical to the plot presented in Fig. 2. The problem is successfully solved.

This procedure is to be used in all cases where the input files contain data points with non-equal spacing.

A problem remains, however, for those data files which are not of ASCII format (e.g. binary files). In such cases, it is advisable to get as much information on the structure of the data file as possible, before proceeding with data manipulation.

APPENDIX

A list of the BASIC-coded program for generating equidistant data points (with included comments) is given below. All relevant information for the users is given within the program.

Program list

```
REM ************************************************************************************
REM *                                                                                  *
REM *                              FILE CONVERTER                                      *
REM *                                                                                  *
REM *        Converts arbitrary ASCII_XY data files into standard LABCALC form         *
REM *                                                                                  *
REM *                                Vladimir Petrusevski,                             *
REM *          Institute of Chemistry, Arhimedova 5, 91000 Skopje, Macedonia           *
REM *                                                                                  *
REM ************************************************************************************

Name1$ = ""    ' ASCII name of original file
Name2$ = ""    ' ASCII name of converted file
```

```
n = 0                   ' Number of data pairs
xa = 0                  ' Particular x of converted file
ya = 0                  ' Corresponding y of converted file
xb = 0: xc = 0          ' x-interval for interpolation
yb = 0: yc = 0          ' y-interval for interpolation
cnt = 0                 ' Counter: index of converted (xa, ya)  pair
s$ = SPACE$(5)          ' Text formator

DIM x(5000), y(5000)      ' Data of original file
DIM x1(5000), y1(5000)  ' Data of converted file
Start:

CLS
PRINT : PRINT
PRINT s$; "                              FILE  CONVERTER"
PRINT  : PRINT
PRINT s$;  "        This is a program for conversion of an arbitrary ASCII X,Y"
PRINT s$;  "data file,  to an  ASCII file standard for use  with  LABCALC. One"
PRINT s$;  "typical example is an  ASCII file where the X-coordinates are not"
PRINT s$;  "regularly spaced (e.g. the output spectrum of DILOR instruments)."
PRINT s$;  "In such cases,  the use of the original files may result in large"
PRINT s$;  "errors (as large as 300 wavenumbers!).  The simplest way to over-"
PRINT s$;  "come the problem is to perform a linear interpolation.  Excellent"
PRINT s$;  "results are obtained for files with closely spaced data points."
PRINT s$;  "       Delete the header  (if there is any) of the input file and"
PRINT s$;  "start with the number of data points.  Proceed with the X,Y pairs"
PRINT s$;  "(these are either arbitrarily spaced or the spacing increases/de-"
PRINT s$;  "creases through the file)."
PRINT
PRINT s$; "                          Press a key to continue ..."

SLEEP
CLS
INPUT "Name of file to be converted = "; Name1$
PRINT
INPUT "Name of converted file = "; Name2$

InputData:

OPEN Name1$ + ".asc" FOR INPUT AS #1   ' opens sequential disk file
                                       ' for input of original data
INPUT #1, n                            ' reads number of data pairs

FOR i = 1 TO n
   INPUT #1, x(i), y(i)                ' and reads the whole spectrum
NEXT i
CLOSE #1                               ' input file Name1$ is closed
```

```
Interpolate:

xa = INT(x(1)): cnt = 1                          ' first x is fixed; counter starts

FOR i = 1 TO n - 1                               ' check all but the last point
   xb = x(i): xc = x(i + 1):                     ' which lies between xb, xc
   yb = y(i): yc = y(i + 1)                      ' its y value being between yb, yc
WHILE xb  >= xa AND xa >  xc                     ' as long as xa is inside the interval
                                                    ' either :
   IF xa = xb THEN                               ' check whether it equals left limit
      ya = yb                                    ' if it does, assign corresponding y
      x1(cnt) = xa: y1(cnt) = ya                 ' write the data point
      xa = xa - 1: cnt = cnt + 1                 ' take next x; increase the counter
   END IF

                                                    ' or :
   IF xb  xa AND xa  xc THEN                     ' check if x is inside the interval
      ya = yb + (yc - yb) / (xc - xb) * (xa - xb)  ' interpolate y
      x1(cnt) = xa: y1(cnt) = ya                 ' write the data point
      xa = xa - 1: cnt = cnt + 1                 ' take next x; increase the counter
   END IF
WEND                                             ' exit if x is outside the interval
                                                 ' and redefine the interval (next i)
NEXT i

cnt = cnt - 1                                    ' ignore last counter value

OPEN Name2$ + ".cnv" FOR OUTPUT AS #2            ' opens sequential disk file
                                                 ' for the converted spectrum

FOR i = 1 TO cnt
   PRINT #2, x1(i)
   PRINT #2, y1(i)                               ' and writes the data '
NEXT i

CLOSE #2                                         ' closes file

END                                              ' and terminates the job
```

Резиме

ЕДНО МОЖНО РЕШЕНИЕ ЗА ПРОБЛЕМИТЕ ПРИ РАБОТА СО LabCalc

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Клучни зборови: трансфер на датотеки; интерполација; спектри

И покрај многуте удобности и моќни команди што ги овозможува, програмскиот пакет LabCalc има еден сериозен недостаток: влезните податоци (бранови броеви, бранови должини и сл.) треба да бидат организирани како множество од еквидистантни точки. Последица на ова е дека голем број ASCII датотеки се неупотребливи во својот изворен облик.

Едно можно решение на овој проблем е да се изврши линеарна интерполација на изворните податоци. Во врска со последново, даден е кус програм во QBASIC, кој овозможува датотеката да биде "преведена" и правилно интерпретирана од страна на програмскиот пакет LabCalc.