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**REPORT: A program for generating method descriptions and bibliographies
of routine work performed in analytical chemistry laboratories.**

by

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1. Introduction

REPORT is an interactive program that allows chemists using routine operational methods to generate short descriptions of the analytical work they performed. The philosophy behind these reports is that they should contain all of the information needed to let a sample-submitter who is not a chemist write the analytical sections of a professional manuscript. The reports are designed to be specific enough that they only describe techniques that were actually performed on the samples, without containing excessive details of laboratory procedures. They do, however, contain the best literature citations that can be quoted in a manuscript to fill in such details. The reports can and should be customized for individual jobs so that they describe any deviations from standard procedures, problems encountered with the samples, and other information that the chemists want to convey to the submitter about the analysis of the samples.

REPORT was written in Lahey fortran F77L-EM/32, and requires an IBM-PC compatible 80486-based computer, or on an 80386 machine with a math coprocessor chip. It contains a built-in DOS extender program, and requires 354K of memory. This program may not run in the presence of other DOS extenders. The sbTeX version of the TeX typesetting program (see below) must also be run to generate reports, and it requires 570K of DOS memory; this is the biggest problem for implementing the REPORT program on most systems. The TeX documentation in the \tex directory (after following the instructions in the Installation section) contains more information on its memory requirements. Note that purchase of this report is in no sense a license fee or purchase fee for the sbTeX program.

The output of the REPORT program is an ASCII file in the TeX typesetting language (.tex file). [TeX is a public domain program that can be freely distributed with the REPORT program. See the TeX documentation for copyright and distribution restrictions.] After a .tex file is created by REPORT, the TeX program is run to convert it into device-independent (.dvi) format. Another public domain program, DVILJ2, is then run to convert the .dvi file into Hewlett Packard printer control language (HP PCL), suitable for printing on HP LaserJet+ or HP LaserJet II (and compatible) printers. The program DVILJ2P can also be run to generate output for HP LaserJet IIp, HP LaserJet III, or HP LaserJet 2000 printers.

The REPORT program is designed to facilitate the making of reports for a large analytical laboratory facility with multiple operational centers. All data files supplied here are the ones used by the authors in the Branch of Geochemistry, U.S. Geological Survey. These may be modified in part, or completely for use elsewhere.

2. Installation

It is assumed in the following directions that you have a basic knowledge of DOS commands. To install the REPORT program and the public domain TeX and DVILJ2 programs on a PC:

- 1) There are two self-extracting archives on the program disk ("rp.exe" and "tx.exe". Extract these to the hard disk with the commands:

b:rp c:
b:tx c:

This will take the archived data files on the floppy disk and extract them to the c: drive (or substitute the letter of another hard disk drive). Directories will automatically be created, if necessary. There may be a conflict there already exists a directory called \tex or \rpt that is used for other purposes than this program.

- 2) Add the directories c:\tex and c:\rpt to the DOS path in the file "autoexec.bat". Also add the line "SET TEXPXL=C:\TEX\DVI-HP" to this file. Reboot the system before running the program.
- 3) If you choose to install on a hard drive other than C:, you will have to reconfigure the tex program. The steps to follow to install on drive D: would be:
 - a) Go to drive D: and change default directory to \tex.
 - b) type "SB38SET". Use the "D" option of this program to change the new drive and path to "d:\tex\formats\" (note slash at end). Exit program.
 - c) type "CD FORMATS" to go to the \tex\formats directory.
 - d) type "\TEX\SB38TEX". Use the "P" option to change the drive to "D:". Exit program.
 - e) Go back to the \tex directory and type "TEX PLAIN". At the "*" prompt, type "\dump" (lowercase!). The program exits.
 - f) Move the file "PLAIN.FMT" to the \tex\formats directory.

3. Generating an analytical report.

Reports are generated in several steps. You would use the following instructions to create a report for a job named "CG01".

3.1) *Running the REPORT program.*

Run the REPORT program by typing "REPORT". You are asked to enter a job number (CG01) and the submitter's name. The job number must be 4 characters long. Several windows then appear on the screen from which information may be selected.

First, select the project name from the left window with the arrow keys. Project names are two-character codes in which the first letter signifies the name of the laboratory where the work was done, and the second letter signifies the general family of methods (e.g., "RT" stands for Reston Trace-element methods). As you change the highlighted project, the available method-description files appear in the 2nd window, and the appropriate analysts for that project appear in the 3rd window. When you have highlighted the correct project, hit <Enter>.

Select the correct method description in the same way from the 2nd window. If the selected project only has one available method, you will be forced to go on to the next step.

Next, select the analysts who did the work from the 3rd window. Use the arrows to highlight the correct analyst, and then hit the spacebar. A check mark appears next to the name. You

may select more than one analyst in this way. When finished, hit <Enter>.

For methods that can run multiple elements, you are now asked to select which elements were run in the rightmost window. By default, all elements are selected with check marks. You can change the selection in the same way as you selected analysts. Both the analyst window and the element window have as their last choice a selection that lets you enter information not on the menu. You can also hit F7 and F8 to select all or unselect all elements, respectively. Again, when you are finished, hit <Enter>. You can now select another project and/or method description.

When you have selected information for all projects and methods that were run, hit the <Escape> key. The REPORT program then makes an ASCII file called "cg01.tex" of your report in the TeX typesetting language.

3.2 Editing the report.

Edit the TeX file if necessary to add any other information you need in the report. Use a text editor that doesn't put binary wordprocessing commands in the file (these will cause TeX to bomb). If you don't know TeX, or you have no manual, try learning by imitation, or ask the authors for help.

3.3 Running the TeX program.

Process the TeX file with the command "TEX CG01" or "TEX CG01.TEX". Output will be a "device independent" file called CG01.DVI. If the TeX program tells you that it needs a missing font (a .tfm file), you may copy these with the network "ftp" program from host labrea.stanford.edu (ip address 36.8.0.47), in its directory /tex/fonts. If your computer is not connected to Internet, ask your local computer expert for help. These files should be put in the \tex\fonttfms directory on your machine. This should only be necessary if you try something fancy in step (2), exploiting your advanced knowledge of TeX.

3.4 Processing the DVI file.

Process the DVI file for printing on an HP LaserJet II printer. Use the command "DVI CG01". This makes a file called "CG01.LJ". You can also send the .lj output directly to your printer with the command "DVI -eLPT1: CG01", in which case you skip step 3.5. The DVI command runs a small batch file in the \tex directory which in turn runs the DVILP2 program. If you want to print on an HP LaserJet IIp, HP LaserJet III, or HP LaserJet 2000 printer, edit DVI.BAT and change DVILP2 to DVILP2P.

If the DVI command tells you that it needs a missing font, FTP it from the same Stanford computer (font files are in its /tex/gf directory). When you find the file on Stanford, it will have a name like "cmti10.300gf". When FTP retrieves it, the name gets truncated to "cmti10.300" on your PC. Translate this file with the GFTOPK utility by typing, "\TEX\GFTOPK CMTI10.300". Next, delete the original file "cmti10.300". Take the newly created file "cmti10.pk", rename it to "cmti10.300" (yes, the same name as the file you just deleted), and put it in your \tex\dvi-hp directory.

3.5 Printing.

Print the LaserJet file using a copy-binary command, i.e., "COPY /B CG01.LJ LPT1:".

4. Changing and adding method descriptions.

The directory \rpt\data should contain all of the data and text files needed to run the report program. All files with the extension .txt contain method descriptions in a special format. Don't edit these without reading the instructions below. These text files are made known to the REPORT program by the file, "files.dat". This ASCII data file associates a two-letter project code with a text file and with a short description that is used as a prompt in the REPORT program. The ASCII file "textop.tex" is copied verbatim to the top of the output file generated by REPORT, and contains TeX formatting information; this file may be edited to change the title and introductory material for the whole report. The ASCII file "ref.tex" contains all bibliographic information. Each reference is written in TeX language and is preceded by a keyword (see below for editing instructions). Finally, the ASCII file "centers.dat" contains the laboratory names corresponding to the first letters of project names.

4.1 Adding a new method description.

- 1) Create a new .txt file in the proper format (described below), and put it in the \rpt\data directory.
- 2) Put a new entry in "files.dat" pointing to the new .txt file. If the first letter of the project name you put in this file is new, add the name of the new laboratory to the file "centers.dat".
- 3) Put any new bibliographic references in "ref.tex" in the proper format (described below).
- 4) Inform the other users of the program of your changes so all can have them.

4.2 Changing a method description.

- 1) Edit the appropriate .txt file with an ASCII editor.
- 2) Put new references in "ref.tex" in the proper format (if any were added).
- 3) Inform the other users of the program of your changes so all can have them.

5. Formats of special ASCII files.

5.1 Method description (.txt) file format.

Part 1: Element list. Method description files must start with a list of elements covered by the method, in the fortran format (I2/10A5/10A5/10A5/10A5), e.g.:

```
12
Na   Pb   Be   Pr   Bi   S   Cl   Pd   Ar   Mo
Ir   Se
```

where, in this case, 12 is the number of elements, and the next two lines list the elements. The REPORT program will let you edit such multiple-element lists interactively in case not all of the elements were determined in a job. The elements *must* be listed like this if you want the list to appear anywhere in the description, separated by commas. The elements also need to be listed like this if you want parts of the description to only appear when certain elements were run. If you don't need either of these features, then the list is superfluous, and you can enter only one element, e.g.:

```
1
Dummy
```

so that the report program will not ask you to edit a list of elements.

Part 2: Title. The next line of the method description file is the title to appear at the top of the report.

Part 3: Text. The remainder of the TXT file is the description of the method in TeX language. Where you want the list of selected elements to appear in the report, place the code "!E". Following the same example given above, the text line,

```
The elements !E were measured by the method of Ozbo (1922).
```

Would appear in the report as,

```
The elements Na, Pb, Be, Pr, Bi, S, Cl, Pd, Ar, Mo, Ir, and Se were measured by the
method of Ozbo (1922).
```

If you want to make part of the text dependent on the presence of one or more elements, you delimit this block of text as follows:

```
!L[Pb/Cl/Ir/Sc]
Blank corrections are made for !N due to their presence in the
technician's fingerprints.
*
```

In this example, the sentence starting with the word "Blank" will only appear in the report if at

least one of the elements, Pb, Cl, Ir, or Sc is in the element list. The !L line delimits the start of the block, the asterisk delimits the end of the block, and both must be on their own lines. The code !N which appears in the block works like !E does above, except that it produces a comma-separated list of the elements in the !L list which are present in the selected-element list. Continuing with the same example, this block would appear as follows in the final report:

Blank corrections are made for Pb, Cl, and Ir due to their presence in the technician's fingerprints.

References: Keywords that point to references in the "ref.tex" file can appear anywhere in the text, each on its own line starting with a % sign. E.g.:

```
%ARUSPJ3SM84A
%BAEDPA2G .89A
```

designates that two references will be associated with this method. Each keyword is 12 characters, excluding the % sign. See below for instructions on creating new references and keywords. If a reference is only to appear if a block of text delimited by !L ... *, then put the reference keyword in that block.

The REPORT program eliminates duplicate references from its output if they appear in more than one section of the report. References will be printed in a separate section at the end of the report no matter where the keywords occur in the text.

5.2 References file format.

The file "ref.tex" contains the references and their keywords. The keywords are designed so that an alphabetical list of them will place the references in the correct order for most journals. The first four characters are the first four letters in the first author's surname. The next two characters are the first author's initials. The 7th character is the total number of authors. The 8th and 9th characters are the initials of the second and third authors' surnames (or spaces if there are less than three authors). The 10th and 11th characters are the last two digits of the year of publication. And, the 12th character resolves cases where the first 11 characters are identical in two references; most references have an "A" in this position.

The file is constructed of keywords on their own lines (starting with a % sign), followed by their references. The reference should start with the characters "\ref", and then appears in TeX language. Part of this file might look like:

```
%ARUSPJ3SM84A
\ref Aruscavage P.J., Simon F.O., and Moore R. (1984) Flameless atomic
absorption determination of platinum, palladium, and rhodium in
geologic materials. {\it Geostand. Newslett.} {\bf 8}, 3-6.
%BAEDPA2G .89A
\ref Baedeker P.A. and Grossman J.N. (1989) {\it The computer} {\it
analysis of high resolution gamma-ray spectra from} {\it instrumental
activation analysis experiments.} U.S. Geol. Surv. Open File Report,
89-454, 88 pp.
```

The order is not important, but it's easier to edit the file if they are alphabetical by keyword.

5.3 *Analysts file format.*

The file "analysts.dat" contains analyst numbers (not currently used by this program), analyst names, and lists of two-letter project codes appropriate for the analysts. The FORTRAN format of each line is (I4, 1X, A25, 30A2). Thus, the line,

```
2366 J.T. Kirk           RTRXLM
```

Indicates that J.T. Kirk, analyst #2366, is a possible analyst on projects RT, RX, and LM. This file can be edited freely, but should be maintained in alphabetical order so that the displayed lists of analysts are also alphabetical.