

doiba Manual

Using PIXE and PIGE to their full
potential with **doiba**

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Introduction

In the early 1980s Eric Clayton developed a software package for the analysis of Proton Induced X-ray Emission (**PIXE**) [6] spectra at the Australian Nuclear Science and Technology Organisation (ANSTO). This package was called **PIXAN** and it is based on work by D.D. Cohen et al. [1, 2] and E. Clayton et al. [3, 4, 5]. The package is optimised for the batch analysis of a large number of similar samples.

It uses a 2 step process to analyse **PIXE** spectra. Command line programs controlled by run control files that contain the parameters of the experiment facilitate the 2 steps of the analysis. In the first step the spectra are fitted using the α - β ratio of the X-ray lines and peak areas are extracted for each element. This step is facilitated by the command line program **batty**.

In the second step the peak areas from **batty** are converted into concentrations using either **thikc** or **thins**. **thinc** uses a thin target approach assuming that sample is thin and the energy loss of the beam as well as the self absorption in the sample are very small. Concentrations calculated by **thins** are reported in ug/cm².

thikc on the other hand does a full calculation of the energy loss of the beam through the sample taking into account the change in X-ray production and self absorption in the sample. Therefore **thikc** requires the sample matrix as an input parameter. The results of **thikc** are reported as mg/kg.

At the same time a peak finding program called **ptanal** was developed at ANSTO, which was used to extract peak areas from Proton Induced γ -ray (**PIGE**) spectra. These can then be converted into concentrations using a reference material.

In 1997 we started developing **dopixe**, a simple graphical user interface for the **PIXAN** package, in order to make it easier to use. Later a separate user interface **dopige** was developed for **PIGE** analysis using **ptanal**. Since most of our analysis uses **PIXE** and **PIGE** simultaneously, both programs were merged into **doiba**. However, as part of the **doiba** package **dopixe** and **dopige** still exist and can be used for individual **PIXE** and **PIGE** analysis.

More recently **doiba** was extended to use **PIXE** and **PIGE** analysis without the need to provide the matrix composition for thick sample analysis. In this mode the results of both the **PIXE** and **PIGE** analysis are used to iteratively calculate the matrix composition. However, **PIXE** and **PIGE** can not determine the matrix composition completely, since a number of elements, namely light elements such as oxygen, nitrogen, carbon and hydrogen can not be measured by either technique.

As a consequence the fraction of these light elements has to be estimated. To estimate the matrix composition using the **PIXE** and **PIGE** results, two different modes have been implemented. In the first mode, the so called iterative mode, all the concentrations resulting from the **PIXE** and **PIGE** analysis are summed. If the sum is less than 100% the missing fraction of the composition is assumed to be made up of the light elements. Since it is not possible to know, how this fraction is divided up into the light elements one of these is chosen. This element is set by the so called **Dark Matter Element**. This name Dark Matter Element was chosen, because is not detected by either **PIXE** or **PIGE**. In most cases this element will be oxygen, but it can be

defined by the user as any other element.

The second mode, the so called oxide mode, calculates the oxygen content from the elements measured by **PIXE** and **PIGE** using the oxide form of these elements. The particular oxide form of each element is defined by the user.

Conventions

The following typographic conventions will be used throughout this text.

Menu Name	PARAMETERNAME
This describes menu items, Menu Name is the name that appears in the GUI, while PARAMETERNAME is the name of this parameter as it is used in the tcl/tk script. The script name is also given here, since it appears in the .rc control files, that can be used to run the interface in batch mode. In the text both will appear as Menu Name and PARAMETERNAME . In contrast a menu item that executes a function appears in the text in the following form Menu Function . In general parameters are referred to by PA- RAMETERNAME throughout the text, because the Menu Name is often shortened, which means it is difficult to decipher their meaning outside of the context in the GUI.	

I GUI Interface

Figure 1 shows the graphical user interface (GUI) of `doiba`. The GUI was designed to show all major **PIXE** and **PIGE** parameters in a single menu. This allows to set up the analysis without the need to switch between menus. The GUI is divided horizontally into sections, which are optically separated by red lines. From the top, the sections are a general setup section, followed by the **PIXE**, **PIGE** sections. It is planned to add another section for **RBS** analysis. The last 2 sections are the experimental setup common to both IBA techniques and a general usage section. At the bottom of the GUI are buttons for all the executable functions.

1 Input Parameters

1.1 General Setup

The general setup section contains is again horizontally divided into two blocks. The upper block contains the entry box for the `PROJECTNAME` and has buttons that allow to load and save the analysis parameters from and to a file. Additionally it shows the current working directory in the right corner. The block below sets parameters such as pathnames, filenames, file extensions and contains controls for batchanalysis as well as the standards used for calibration.

Project Name	PROJECTNAME
--------------	-------------

This variable is used as a tag for the analysis and is used throughout the various steps of the analysis to generate the filename of the output files. During analysis a number of files are generated that contain either analysis results or record the analysis parameters. They provide a record of the analysis that has been performed and allow the user to review the analysis parameters or recall them into the program at a later time. The names of these files take the general form `PROJECTNAME.ext`, where `ext` indicates the type of data in the file.

An exception from this rule are `csv` files, that can be directly imported into Excel. Since the extension has to be `csv` in this case, the identifier that determines the content, is append onto the filename itself.

The `PROJECTNAME` variable is created automatically from the current date whenever `doiba` is started. It takes the form `ddmmmyy` or `05feb08` in the example of figure 1. Once the program is started it may be changed by the user.

Generally there are two different types of files, result files and parameter or run control (`rc`) files. Run control files are created, whenever the program executes a part of the analysis or a calibration. Since the analysis is a multi-step process and parameters can be changed between different steps, parameters are saved at each step to provide

1 INPUT PARAMETERS

PIXE & PIGE Analysis

PROJECT NAME :	05feb08	rc-Files	STO-rc	RCL-rc	chdir	/home/msAINSE/A.Smith	
PXE Archive	<input type="checkbox"/>	Core	pixe	Ext	rpt	Path	pixe
PIGE Archive	<input type="checkbox"/>	Core	pige	Ext	rpt	Path	pige
<input checked="" type="checkbox"/> use batch <input type="checkbox"/> batchfile Run-Numbers(Standard) 3(A#16565) 4(CaF ₂ -#9622) 5(0							
PIXE DETECTOR : Energy Calibration: gain 0.019900 keV/chn offset -0.050000 keV X-Ray Detector : ORTEC 8-1579							
thick Be	0.3000 μm	thick Si(dead)	0.0200 μm	thick Au	4.2600 mm	Thick Si	0.8300 μm
Layer #1 Mylar	0.048800 mm	Filtermaterial	thickness	Fraction Hole Area	clear	Distance	99.00 mm
Layer #2 Perspex	1.840000 mm			custom	Mode 2	ENORT	1 NORD 4 POLY(l=0,NORD) 0.1000 0.
Layer #3 none	0.000000 mm			GMB-PinHole	Mode 3	ENORT	1 NORD 4
Layer #4 none	0.000000 mm			Alex-PinHole	Mode 5	CURV	1.001000 ISP 2
Layer #5 none	0.000000 mm			Old-PinHole	FITMODE :	IFITX	1
LIST OF ELEMENTS : SUMPEAKS: BATTY ANALYSIS PARAMETER : BATTY FIT PARAMETER :							
Al Si P S C K Ca Ti V Cr Mn Fe Co I		3	Emin 1.20000 keV Emax 25.0000 keV Cutoff 0.20000 MeV	0.05000 0.00300 0.00300 1.00000			
PIGE OFF DETECTOR : Energy Calibration: gain 4.0085 keV/chn offset -3.5242 keV q-Ray Detector : NewFred Effic. 50 %							
Det. Diam.	67.5 mm	Thick (Ge)	71.0 mm	Distance	91.0 mm	Start Fit	40 chn Width 4 chn STDV 2 Search Width 5.0 keV
Beam Energy	Total Charge	Main Components :	NA AL SI CA K FE O	Matrix :	Thick	Thin	Exp. Err.: 10 %
12.501 MeV	20 μC	Concentrations :	3.23 6.79 34.30 0.89 3.63 1.78 39.14	fixedInput	C in Thick :	20 %	Cal. Err.: 5 %
Beamlne :	SR2	Customer :	A. Smith	Analysis :	Printer :	b53sr2	
<input type="checkbox"/> Run Battty Ctrl+E <input type="checkbox"/> Run Conc Ctrl+T <input type="checkbox"/> Calibrate PIXE <input type="checkbox"/> Calibrate PIGE							
<input type="checkbox"/> Convert Files <input type="checkbox"/> Archive Files <input type="checkbox"/> File Viewer <input type="checkbox"/> Make Report <input type="checkbox"/> Edit Batch <input type="checkbox"/> Plot							

Figure 1: Graphical user interface of doiba.

a complete record for later review. The extension of run control files generally ends in **rc**.

Historically there are a separate run control files for **PIXE** and **PIGE** parameters. This structure has been kept to be able to run **doiba** or **dopixe** and **dopige** individually on the same data set with all of them accessing the same parameters.

Run control files, with an extension starting with an X contain the all **PIXE** parameters, while the ones starting with G contain the **PIGE** parameter set. Extensions starting with I contain both parameters sets. Whenever the program is started it searches for the most recent version of the run control file and loads its parameters. In this way an analysis can be interrupted at any stage and continued later with the parameter set in the last analysis step executed. However, changing a parameter does not automatically save the new parameters, they only get saved when one of analysis steps are executed.

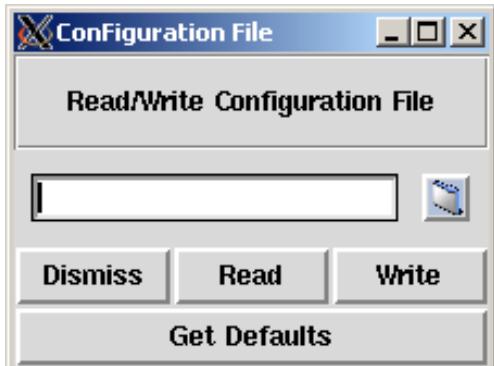
Since the the parameters are saved in the analysis directory, it is recommended to use a separate directory for each analysis. In this case the parameter set last used for a particular analysis is automatically loaded whenever **doiba** is started in its directory.

In parallel a file **.LastPIXE.Xrc** or **.LastPIXE.Grc** is saved in the users home directory. These files are read whenever there are no **rc** files present in the current directory. In this way the last parameter set is always reloaded even if a new set of samples is analysed.

It is also possible to read previous parameter sets or temporarily store parameters sets, using the buttons in the top section. These are described in the following.

rc-Files

Next to the field for the **PROJECTMANE** are 3 buttons for loading and writing of the **doiba** parameters from or to a file. To reload a parameters set from a previous analysis or save the parameters at any stage the button **rc-Files** is provided.



Clicking on **rc-Files** the field brings up the Configuration File box. In the entry box either enter the name of the configuration file directly or select a file by pressing the button to right of the entry window. This lets you select a configuration file starting from the current working directory.

The **Get Defaults** button selects the data directory, that contains a number of **PIXE** and **PIGE** configuration file examples. After selecting a files press **Read** to read the parameters into the Menu.

Figure 2: Configuration file menu window.

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STO-rc and RCL-rc

These two buttons allow to temporarily store and recall the values in the menu. **STO-rc** will save all the parameters in a temporary file, while **RCL-rc** will recall them. However, **RCL-rc** will only recall the values from the last **STO-rc** command. These functions are intended to temporarily store parameters after a good solution for the analysis has been found and one subsequently tries to improve on this analysis. If the analysis, however, does improve the stored parameter set can then easily be retrieved.

Spectra Names

The second block of the top section is vertically divided into 3 sections. The left section defines the filename and pathnames for each of the analysis techniques. The spectra filename has to be of the following format **core###.ext** where **core** and **ext** can be any string, while **###** has to be a 3 digit number. The **Path** gives the path where the spectra are expected. Since the program combines **PIXE** and **PIGE**, it is recommended to place the data from the different techniques in their own subdirectories. Although this is not mandatory, it will make it easier to select the result files, specially when hundreds of spectra are being analysed.

Spectrum files have to be provided in special ASCII format for analysis. The listing shown below shows the format used by the underlying programs **batty** and **concs**. The first line of data files is a comment with a maximum of 80 characters. However the first item in this line has to be of the form **RUN=001** where **001** can be any 3 digit number from **001** to **999**. **RUN=001** has to be followed by a blank space. The second line has to contain at least 2 numbers, where the first number is interpreted as the block number, which is an identifier for the spectrum and the second number gives the number of data points in the data file. These 2 lines are followed by the data, which are arranged as 9 data points per line.

Example of the minimal spectrum file format.

RUN=001 pixe Nov07 CUSTOMER				1/11/07 10:15:30 AM				
1001	2048							
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	17	28	29
27	22	25	26	18	27	27	23	25
23	23	22	21	29	24	16	16	23
26	15	26	28	19	28	24	23	29
18	20	33	30	27	17	27	40	41
61	66	71	79	98	105	112	143	178
272	422	714	856	1132	1366	1520	1348	1142
976	684	492	312	199	142	92	81	66
67	50	61	49	42	49	53	54	55
49	51	44	46	59	58	59	49	53
51	42	63	60	60	60	63	58	69
66	80	91	96	117	99	104	93	104
106	96	98	95	95	77	75	75	104
106	95	96	87	106	95	98	111	105
102	107	153	188	249	397	729	1186	1850
2575	3613	4296	4933	4990	4620	4077	3288	2400

1.1 General Setup

For **doiba** this simple data format has been extended with additional parameters. The listing below shows an example of the extended format, that can be interpreted by **doiba**. It used additional data in the second line to read the **SAMPLENAME**, the format of which has to be of the form **SAMPLE=SAMPLENAME**. The **SAMPLENAME** can not contain any blanks or TABs. A separate command line tool **extract-batch**, can be used to generate a batchfile from all the datafiles in a directory, which have to be of the extended format described below. This batchfile can be used with **doiba**.

Example of the extended spectrum file format.

RUN=001	pixe	Nov07	CUSTOMER		1/11/07	10:15:30	AM
1001	2048		SAMPLE=NBS278	POSITION		15.00uC	12:26:39
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	17	28
27	22	25	26	18	27	27	25
23	23	22	21	29	24	16	16
26	15	26	28	19	28	24	23
18	20	33	30	27	17	27	40
61	66	71	79	98	105	112	143
272	422	714	856	1132	1366	1520	1348
976	684	492	312	199	142	92	81
67	50	61	49	42	49	53	54
49	51	44	46	59	58	59	49
51	42	63	60	60	60	63	58
66	80	91	96	117	99	104	93
106	96	98	95	95	77	75	75
							104

Archives

batty and **concs** were designed to analyse a large number of spectra, which are contained in a single file. Such a file is called an archive with the spectra simply catenated into a single file. However, this feature is no longer used by **doiba** and spectra stored in such an archive have to be extracted. In order to accommodate such large archive files the **Archive** entry can be used. The file can either be entered directly in the entry field or through the button at the right. If it is entered through the file-selection box it will be automatically extracted. An archive can be compressed with zip and the program will recognize this and handle the file accordingly. The extracted files will be saved as **PATH/CORE/###.a-rpt** e.g. **dir/pixe001.a-rpt**. If **PATH** does not exist the path will be created automatically. The number for the filename will be taken from the expression **RUN=###** which appears in the first line of each file header. In order to avoid overwriting existing spectra the extract program changes the extension of the spectra to **a-rpt**, which marks them as extracted from an archive. When the program is terminated and **clean up** is selected extracted spectra will automatically be removed.

Batch Analysis

The middle block of the top section is used to select, which files will be analysed by **batty** and **concs**. Two different modi are possible, the first uses a batchfile, while the second simply analyses all files with numbers in the range from first to last. The

1 INPUT PARAMETERS

tick-box *use batch* selects if the batchfile is used in the analysis. When the tick-box is set, the script will analyse spectra in the order listed in the *batchfile*. Otherwise the script searches sequentially for files with numbers between *first* and *last* given in the entry below.

batch file	BATCHFILENAME
------------	---------------

An example of the batchfile is given in the entry box below. Any lines starting with a # are comments and will be ignored. In the minimum configuration the batchfile consists of 2 columns, the first containing the number in the file name (CORE/###.rpt), while the second is the sample name to be used in the analysis.

Some analysis parameters can vary from sample to sample. Therefore the batchfile provides a way to set them individually for each spectrum. This is done by special commands which use the syntax, *COMMAND: value[s]*. Three special commands, *CHARGE:*, *COMP:* and *CARBON:* are available.

The commands *CHARGE:* and *CARBON:* define the total charge of the analysis (in μC) and an optional carbon content (in percent) in the sample. In both cases the value is a number without the units. The command *COMP:* defines the matrix composition of the sample to be used in the analysis. This command is followed by a number of element concentration pairs, with the concentration given in percent.

These commands can appear in any order, but have to follow the run number and sample name in the same line. Any values set with these commands will apply for the current spectrum as well as any subsequent one. In this way they act as switch that changes the parameters from this point forward. If any of these parameters are set in the batch file they should also be set for the first sample of the batch file. Otherwise the parameters from the menu will be used for the first sample.

Example of batch file, lines beginning with # are comments.

```
#  
#   batch file for sample analysis 12. Dec 2007  
#  
001      NBS278-20%,00  CHARGE: 10 CARBON: 0 COMP: NA 3.2 AL 6.8 ...  
002          NBS278  CHARGE: 20  
#   new matrix composition for following samples  
003          WBS298  COMP: SI 22.80 AL 14.30 MN 0.02 MG 0.45 ...  
004          ABT306  
#   again a new matrix composition for following samples  
#   additionally samples were mixed with 20% graphite  
020          C1045_10 CARBON: 20 COMP: SI 6.0 AL 3.0 FE 1.0 ...  
021          CR202  
022          CBT230  
023          CBT231  
024          CBT232  
#   new matrix composition, samples mixed with 20% graphite  
030          NBT330 COMP: 0 48.88 NA 0.15 AL 9.89 SI 30.79 ...  
031          NBT331  
032          NBT332
```

Standards

Run-Numbers(Standard)	<i>STANDARDSTRING</i>
-----------------------	-----------------------

During calibration for both **PIXE** and **PIGE** only selected spectra, normally of standard reference materials, are analysed. Which spectra are analysed is defined by *STANDARDSTRING*, which is entered in this box. The format of the string is **nn,nn(Standard)** for example

1,13(NBS278) 2,14(ORC)

This means that the files `core001.ext` and `core013.ext` are analysed and compared with the standard NBS278, while the files `core002.ext` and `core014.ext` are compared with the standard ORC. The standard has to be included in the standard data base (*Standardfile*), in which the composition as well as the certified values are stored.

The *List of Standard Spectra* can automatically be extracted from the batchfile. This can be done by placing the cursor in the batch file entry box and pressing enter or pressing the button below the standard string. This will read the batchfile and search for sample names that are identical to names in standard data base and then create the list automatically. However, the name of the standard has to match the the name in the data base exactly, with the match being case sensitive.

To allow standards being given individual identifiers in order to track them, the standard name can be extended by such an identifier. The identifier and the sample name have be separated by a comma, for instance NBS278,A1 means this is the sample A1 of the standard NBS278. When the batch file is evaluated this sample will still be identified as standard NBS278.

1.2 PIXE Parameters

The second section of the menu contains all the parameters for the **PIXE** analysis. The parameters are divided into four groups, which appear in the GUI in the top section, a left and right middle section and a section in the bottom part, which itself subdivides into many smaller parts. The top block of this section contains all detector parameters, while the central part contains the filter parameters on left and the background settings on the right. More parameter controlling the fitting of the X-ray spectra are in the bottom of the **PIXE** section.

Detector Parameters

gain	<i>ENERGYSLOPE</i>
------	--------------------

ENERGYSLOPE is the slope or gain of the energy calibration of the **PIXE** spectra given in keV/channel.

1 INPUT PARAMETERS

offset

ENERGYOFFSET

ENERGYOFFSET is the offset of the energy calibration of the **PIXE** spectra given in keV.

X-Ray Detector

The **X-Ray Detector** pull down menu can be used to set all detector parameters for detectors predefined in the beamline configuration file. An example for the detector definition section of the beamline file is shown below. The beamline file is located in the data directory of the **doiba** package. Not all detector parameters have to be defined in the detector definition file. If the distance of the detector from the target can be varied, it may be useful to not define this value here.

Example of definition file for X-Ray detectors.

```
X-rayDetector:      ORTEC 8-1579
  DetectorDiam:    4.0000
  DetectorWindow:  25.000
  DetectorThick:   4.2600
  AuThick:         0.0200
  DeadThick:       0.3000
  FG:              0.8300

X-rayDetector:      Canberra 0502846
  DetectorDiam:    11.300
  DetectorWindow:  25.000
  DetectorThick:   10.0000
  AuThick:         0.0200
  DeadThick:       0.3000
  FG:              1.0000
```

thick Be

DXBE

DXBE is the thickness of the Be window in μm in front of the detector. The value is typically $25\mu\text{m}$ for a **PIXE** detector. However, detectors designed for electron microscopy may have a thinner window, or even a window made of a different material. In this case the filter section has to be used to define the detector window.

thick Si(dead)

DXSI

DXSI is the dead layer thickness of the detector crystal in μm . Values between 0.100-0.300 μm are typical for SiLi detectors.

thick Au

DXAU

DXAU is the thickness of the gold contact on the front of the detector crystal in μm . This layer is quite thin and is typically 20 nm thick.

1.2 PIXE Parameters

Thick (Si)	<i>DTHIK</i>
-------------------	--------------

DTHIK is the thickness of the detector crystal in mm. The current code only uses efficiencies for Silicon, thus limiting the program to Si based detectors.

FG	<i>DFG</i>
-----------	------------

DFG is the Detector Geometry Factor. It has a value smaller or equal to one. This value is experimentally defined and has a value of 0.83 for our detector. In many case it will be sufficient to set this value to 1.0.

Thick Ice	<i>DXICE</i>
------------------	--------------

DXICE is the thickness of the ice layer on the front surface of the detector in μm . This layer tends to build up over the year, unless the the detector is pumped regularly.

Distance	<i>DISTANCE</i>
-----------------	-----------------

DISTANCE is distance of the detector crystal from the surface of the sample in mm.

Incident Angle	<i>BEAMANGLE</i>
-----------------------	------------------

BEAMANGLE is the incident angle of the beam onto the target.

Detector Angle	<i>DETANGLE</i>
-----------------------	-----------------

DETANGLE is the angle of the detector relative to the incoming beam, in degrees.

Detector Diam	<i>DETSIZE</i>
----------------------	----------------

DETSIZE is the diameter of the detector given in mm, assuming a circular geometry of the detector.

Filter Parameters

The filter parameters are used to define a filter or absorber placed in front of the X-ray detector. This filter can be quite complicated and can consist on up to 5 different layers. Each layer is defined by the material, the thickness and an optional hole in the centre. The material the layers are made off is limited to Mylar, Perspex, Kapton, beryllium, graphite, aluminium and air. However, these are the most commonly used materials and this selection should be sufficient for most cases. Air has been included as a filter material to allow the program to be used for the analysis of spectra taken with an external ion beam.

A filter material is selected by selecting one of the check-boxes with the material. This enters the material into the first layer of the filter list and also selects the unit used for this material. For all filter materials the thickness is given in mm except for Be for which the thickness has to be entered as μm . When another material type is

1 INPUT PARAMETERS

selected all the material types are moved down the stack, which means material of layer 1 becomes material of layer 2 and so on. When the check-box clear is selected, all the filter input parameters are cleared.

In order to define a composite filter with more than one layer, custom has to be selected. However, the materials list has to be built up first by selecting the various materials in the correct order and moving them down the list. Once custom has been selected the thickness and Hole Area values can be entered for each material.

Three custom filters have been predefined, however, they can be redefined in the file `filter.config`. An example of this file is shown below.

Example of filter definition file used to redefine custom filters in **doiba**.

```
set C1FILTERNAME          "MyPinhole1"

set C1FILTERNUMBER(1)      1
set C1FILTERNUMBER(2)      2
set C1FILTERNUMBER(3)      0
set C1FILTERNUMBER(4)      0
set C1FILTERNUMBER(5)      0

set C1FILTERTHICK(1)       0.048500
set C1FILTERTHICK(2)       2.300000
set C1FILTERTHICK(3)       0.000000
set C1FILTERTHICK(4)       0.000000
set C1FILTERTHICK(5)       0.000000

set C1FILTERHOLE(1)        0.000000
set C1FILTERHOLE(2)        0.100000
set C1FILTERHOLE(3)        0.000000
set C1FILTERHOLE(4)        0.000000
set C1FILTERHOLE(5)        0.000000

set C2FILTERNAME          "MyPinhole2"

set C2FILTERNUMBER(1)      1
set C2FILTERNUMBER(2)      2
set C2FILTERNUMBER(3)      0
set C2FILTERNUMBER(4)      0
set C2FILTERNUMBER(5)      0
.
.

set C3FILTERNAME          "MyPinhole3"

set C3FILTERNUMBER(1)      1
set C3FILTERNUMBER(2)      2
set C3FILTERNUMBER(3)      0
set C3FILTERNUMBER(4)      0
set C3FILTERNUMBER(5)      0
.
```

Background**BACKGROUND**

The major contributor to the background in the region from 1 to 10 keV is secondary electron bremsstrahlung and this background has to be subtracted before the fitting. This section defines how **batty** handles background subtraction. There are 4 different modes of which modes 1 and 5 are probably the most useful. The first is a simple background subtraction using a background spectrum given in a file. Modes 2 and 3 use a polynomial estimated from the spectrum while mode 5 uses an approach based on a peak filling algorithm.

Mode 1**1**

The first mode is a simple subtraction of a fixed background spectrum. The name of this file has to be entered in the **Background Filename** field. The background spectrum is given in a histogram format, similar to the data file format read by **batty**. The channels in the background spectrum have to align with the channels in the spectra to be analysed. However the intensity in each channel is given as a floating point value instead of an integer, to allow for higher sensitivity. Because of the floating point representation only 6 channels are given per line instead of 9 numbers in the spectrum files. An example of the format is shown below.

Example of background file.

Background Spectrum for 2.5 MeVp on thin C 40uC -max 80 characters					
22	750				
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.1	0.3	0.6	1.2
2.3	4.1	7.2	11.8	18.8	28.8
42.8	61.5	86.1	117.5	156.6	204.3
261.1	327.7	404.3	490.9	587.4	693.5
808.5	931.6	1061.9	1198.4	1339.9	1485.2
1633.1	1782.4	1932.1	2081.0	2228.2	2372.7
2513.9	2651.1	2783.6	2911.2	3033.3	3149.9
3260.7	3365.6	3464.7	3558.0	3645.4	3727.3
3803.6	3591.7	3660.5	3724.7	3784.4	3839.7
3890.7	3937.7	3980.7	4020.0	4055.5	4087.5
4116.1	4141.3	4163.4	4182.3	4198.2	4211.2
4221.3	4200.5	4165.6	4121.3	4066.8	3995.9

Mode 2**2**

In mode 2 the background is modeled using an Nth order polynomial of the form

$$Back(E_i) = S \exp \sum_{k=0}^N a_k (E_i - E_0)^k \quad (1)$$

where S is the term that describes the detector efficiency and self absorption. The order of the N (**NORD**) and the constant E_0 (**ENORD**) are entered into the two adjacent fields. The next field contains the $N + 1$ coefficients of the background polynomial a_k . These values have to be separated by blank spaces.

1 INPUT PARAMETERS

Mode 5

5

Mode 5 defines a using a peak filling algorithm. Although it is not as smooth as a polynomial fit, it reliably produces a usable background in most cases. This background is defined by the curvature *CURV* and low energy spacing *ISP*. Values of 1.001 for *CURV* and 2 for *ISP* produce good results for the background for most spectra.

IFITX

IFITX

IFITX determines how the background is used in the least squares fit.

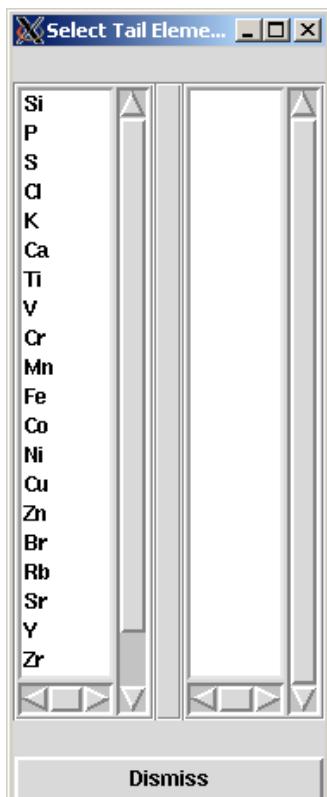
IFITX=1 The background is left fixed.

IFITX=2 The background is scaled, i.e. the shape is maintained but it's magnitude is varied during the fit.

IFITX=3 The polynomial parameters a_k of equation 1 are varied as part of the fitting procedure. If the background mode is 5 (*IBAK*=5) *IFITX* is automatically reset from 3 to 2.

ITAIL

ITAIL



ITAIL is a list of elements with an exponential tail distorting the Gaussian peak. The elements in this list can not be entered manually. To select tail elements double click on the field and the window Select Tail Elements shown in Figure 3 pops up, with the elements of the shopping (see **LIST OF ELEMENTS**) list in the left pane and the tail elements on the right.

To select an element double click on the element in the left list and to de-select an element double click the element in the right list.

LIST OF ELEMENTS

ELEMENTS

ELEMENTS is the list of elements the PIXE spectra are analysed for, which is often referred to as shopping list. The elements can be given in lower or upper case, although, *batty* requires upper case. (The list is converted internally by *doiba*.) If the list is entered by hand a simple element name such as Ca refers to the k-lines, while, PbL means the l-lines for lead.

Double clicking on the input line will bring up a periodic table, from which the elements can be selected. In the table k-lines are selected with the left mouse button, l-lines with the middle mouse button and m-lines with the right one.

Figure 3: Tail element selection window.

1.2 PIXE Parameters

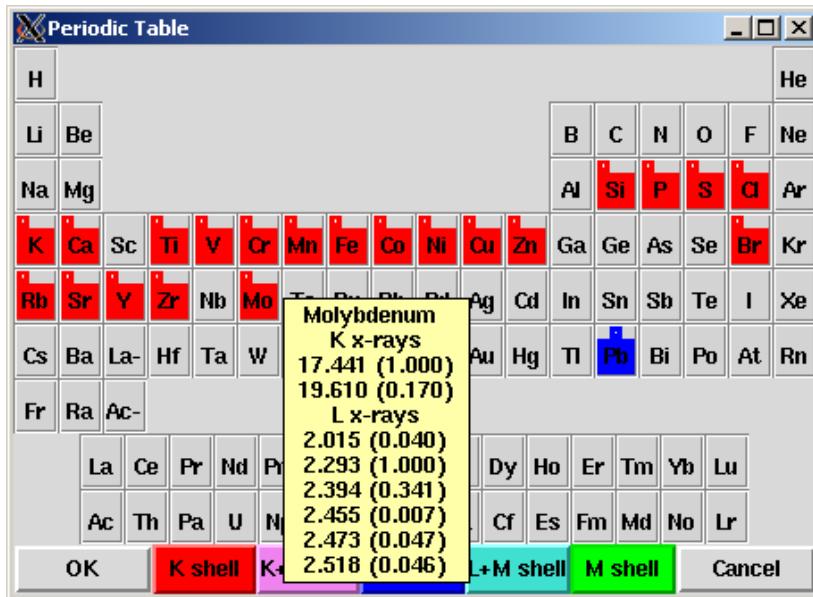


Figure 4: Periodic Table window to select elements for **PIXE** analysis.

Hovering over an element, with the mouse will display a list with characteristic x-ray energies for this element. This list shows both the x-ray energies and relative intensities of the lines. The data is extracted from `dset2` file, which is used by the analysis.

SUMPEAKS

SUMPEAKS

If this number is greater then 0 an additional element called `SUME` is added to the shopping list. The characteristic energies for this element are calculated as sums of the highest energy peaks. `SUMPEAKS` is the number of elements to be included in the calculation of energy positions and relative intensities for this element (`SUME`).

Batty Analysis Parameters

Emin

ENERGYMIN

`ENERGYMIN` is the lower limit for the `batty` fit.

Emax

ENERGYMAX

`ENERGYMIN` is the upper limit for the `batty` fit.

Cutoff

ECUTOFF

The concentration of an element is calculated by integrating the x-ray yield over the range of ion beam. This takes into account the changing x-ray yield as the beam

1 INPUT PARAMETERS

energy decreases, while the ion is penetrating deeper into the material. It also takes into account the increased self-absorption of x-rays generated at greater depth. As a consequence of both effects the contribution to the x-ray yield decreases with depth or ion energy. To save processing time a low energy cut off **ECUTOFF** is defined, that sets the low energy limit in the x-ray yield calculation. This parameter has no effect for thin sample calculations. However, it can be used to simulate samples with an intermediate thickness.

Batty Fitting Parameters

These parameters are used to control the fitting parameters in **batty**. The values are optimised and should not be changed.

1.3 PIGE Parameters

This section contains the parameters controlling the **PIGE** analysis. The check-box is used to switch the **PIGE** analysis on or off. The status is indicated by display above the check-box, which shows either **PIGE ON** or **PIGE OFF**. If **PIGE** is **ON** **PIGE** is automatically included in the analysis.

A number of parameters in this section are not activated yet. The input area for these parameters is gray and input has been disabled. These parameters are intended to allow comparison of **PIGE** calibrations independent of the γ -ray detector efficiency and detector geometry.

Energy Calibration

This sets the energy calibration for **PIGE** spectra and is used by **ptanal**. Note the energy calibration parameter names in the run control files are the same for **PIXE** and **PIGE**. However, internally the variables are different and because their values are read from different control files, there is no risk of them being mixed up. Nevertheless care has to be taken when the run control files are used to set the parameters.

gain

ENERGYSLOPE

This is the slope of the energy calibration of the spectrum given in keV/channel.

offset

ENERGYOFFSET

This is the offset of the energy calibration of the spectrum given in keV.

g-Ray Detector

The **g-Ray Detector** pull down menu can be used to set all detector parameters for detectors predefined in the beamline configuration file. An example for the γ -ray detector definition section of the beamline file is shown below. The beamline file is located

1.3 PIGE Parameters

in the data directory of the **doiba** package. Not all detector parameters have to be defined in the detector definition file. If the distance of the detector from the target can be varied, it may be useful to not define this value here.

Example of definition file for γ -detectors.

```
G-rayDetector:      NewFred
GEfficiency:       58.500
DetectorDiam:     67.500
DetectorThick:    71.000

G-rayDetector:      BIGFred
GEfficiency:       40.000
DetectorDiam:     64.100
DetectorThick:    57.500
```

ptanal peak analysis parameters

Det. Diam

PIGEDETDIAM

PIGEDETDIAM is the diameter of the **PIGE** detector.

Thick (Ge)

PIGEDETTHICK

PIGEDETTHICK is the thickness of the **PIGE** detector.

Distance

PIGEDISTANCE

PIGEDISTANCE is the distance of the **PIGE** detector from the target.

Effic

PIGEEFFICIENCY

PIGEEFFICIENCY is the efficiency of the **PIGE** detector.

Start Fit

PIGESTARTCHANNEL

PIGESTARTCHANNEL is the channel in which **ptanal** starts the peak search.

Width

PIGEMINWIDTH

PIGEMINWIDTH is the minimum width for peaks. Peaks with a smaller width are discarded by **ptanal** as noise.

STDV

PIGESTDV

PIGESTDV is the minimum standard deviation for peaks. Peaks with a smaller area are discarded by **ptanal** as noise.

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Search Width	PIGEDELTA
<p><i>PIGEDELTA</i> is the search width for a peak. If a peak is found within this distance of the characteristic energy it's area is used to calculate the concentration for this element. If the energy calibration is not accurate, characteristic peaks may be discarded if the value for <i>PIGEDELTA</i> is too small.</p>	

1.4 Experimental Setup

This section contains parameters common to all **IBA** techniques. This assumes that the different techniques have been applied simultaneously and that these parameters are indeed the same. The program is mainly intended for these types of analysis and it can at this stage only be used in cases where the common parameters are the same for the all **IBA** techniques.

Beam Energy	BEAMENERGY
<p><i>BEAMENERGY</i> is the energy of the ion beam in MeV.</p>	

Total Charge	TOTALCHARGE
<p><i>TOTALCHARGE</i> is the total accumulated charge used in the analysis in μC.</p>	

Matrix Composition

In the standard mode the matrix composition of the sample is required for both **PIXE** and **PIGE**. In **PIXE** the composition is used to calculate the energy loss of the beam in the sample and the self absorption of X-rays.

In the iterative and oxide mode the composition is calculated using the **PIXE** and **PIGE** results. In this case the 2 fields (*CompELEMENTS* and *ConcELEMENTS*) have to be empty, otherwise elements in these fields are added to the calculated composition.

Main Components	CompELEMENTS
<p><i>CompELEMENTS</i> is the list of the major matrix elements of the analysed sample. Although in principle elements with ppm concentrations can be included in this list, it is not useful to include elements with concentrations smaller than 0.1%.</p>	

Double clicking on the entry window will bring up a window with a list of materials. A material can be selected by double clicking the name. (see materials file in Sect. 3.3) A standard composition for this material will then directly be entered into this and the following field.

Concentrations	ConcELEMENTS
<p><i>ConcELEMENTS</i> is a list of the concentration (in %) of the major matrix element in the same order as the elements in <i>CompELEMENTS</i> in the entry above.</p>	

1.4 Experimental Setup

Double click the entry box and the `dochemistry` window will open. This allows to convert chemical formulas in concentrations. (see Sec. 6.6)

Matrix

The Matrix field is used to select the method used to calculate the matrix composition. Three different methods can be selected; `fixed/input`, `iterate` or `oxide`. Clicking the field with the selection will change the selection. When `fixed/input` is selected the input matrix in the fields **Main Components** and **Concentrations** is used. If any of the other two methods are used these fields should be kept empty and the matrix is calculated from the **PIXE** and **PIGE** results. These 2 methods are described in more detail in section 2. The selection in this field only applies to thick sample analysis.

Thick or Thin samples

The **PIXAN** package uses two different approaches to calculate concentrations from peak areas. One assumes a thin sample, in which case self absorption in the sample and the energy loss of the ion beam in the sample are small. This is the case for very thin layers of material on a light matrix, such as a polymer film or graphite. An example for this are fine particles collected on a filter material. In this case concentrations are calculated in ng/cm^2 .

The second approach uses a full thick sample calculation, which takes into account the beam energy loss and self absorption in the sample. In this case the results are given in mg/kg . These samples can be solid samples or pressed powders. Pressed powders are sometimes mixed with graphite to make them conductive, but also to make it easier to press them into pellets. To account for this type of sample an extra parameter has been added, which adds a fixed amount of graphite to the samples.

The same can be achieved by adding the graphite to the matrix composition. However, in this case the results computed by `doiba` are for the pure sample before the graphite was added, while the results calculated in the latter case are for the sample including the graphite.

Errors

The errors resulting from the spectrum analysis include only statistical errors due the fitting and background subtraction. However, this does not include systematic errors in calculation of the **PIXE** concentration due to uncertainties in excitation cross section, beam energy loss etc. Therefore two parameters `ERROREXPER` and `ERRORSTAND` are added to account for these additional sources of uncertainty.

Exp. Err.

ERROREXPER

`ERROREXPER` is to account for systematic errors due in the theoretical parameters, used to calculate cross sections and absorption of the x-rays.

2 EXTRA MENUS

Cal. Err.	ERRORSTAND
-----------	------------

ERRORSTAND is supposed to account for systematic errors due to experimental parameters, such as uncertainties in the detector distance and the filter parameters.

1.5 General Parameter

This section contains general parameters that are used to control the operation of **doiba**. The first field in this section allows to select a beamline. If there are different beamlines or experimental setups used in a laboratory, then the parameters for these can be recorded in a file. The set of parameters for each beamline can then be set by selecting the beamline in this field. The parameters are stored in the file **beamlines**.

Example of definition file for beamlines.

```
Beamline: MP
X-rayDetector: Canberra 0502846
Distance: 33.00
DetectorAngle: 45.00
G-RayDetector: NONE

Beamline: SIBA1
X-rayDetector: ORTEC 8-1579
Distance: 98.00
DetectorAngle: 45.00
G-rayDetector: NewFred
Distance: 179.00
DetectorAngle: 45.00
```

Customer

CUSTOMER is used to enter the name of the customer for whom the analysis was performed. This name will appear in the final PDF output document as customer.

Analysis

ANALYSIS is used to enter the date when the analysis was performed. This parameter is used in the PDF output file.

2 Extra Menus

Most parameters that are required for the analysis can be set in the main menu. However, there are 3 extra menus, the plot menu, the options menu and the iterative menu, in which analysis parameters can be set.

Plot Menu

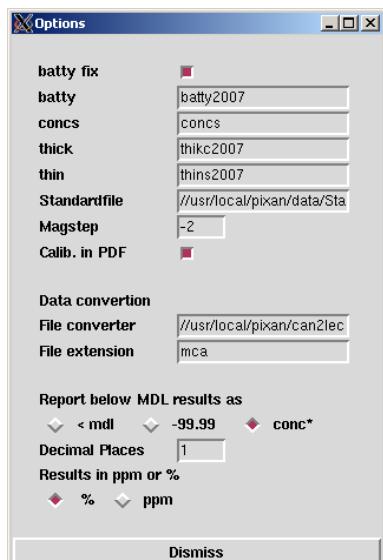
This menu can be accessed through the **Plot** button at the bottom of the GUI. The Plot Menu has been made somewhat obsolete by the new File Viewer **fv**, which can display spectra as well as the batty fit results interactively. **fv** will display rpt and plot files and has a much more direct response to scale changes, compared to plotting routines of **doiba**, which creates a postscript file from the data. However, the postscript plots created from the settings of this menu are included in the final report file, and therefore the values should be chosen so that the full spectrum is shown.

This menu allows to set the plot region for the spectra, for each **IBA** technique. Minimum and maximum values as well as the distance of the tics can be set for both X and Y axis. For both axis linear or logarithmic scales can be selected. In the latter case the tics are set automatically. For the y axis the maximum value can be left blank, in which case the maximum is chosen automatically and will vary from spectrum to spectrum.

All spectra are plotted and written to a postscript file after the fitting and peak finding has been completed, which means plotting ranges have to be chosen before the fitting. However, the spectra can be re-plotted using the Replot function. In this case all the spectra of the analysis are re-plotted, which will take some time.

By default the Y axis is set to logarithmic and Y-max value is left blank, which means this value adjusted automatically for each spectrum. For **PIXE** spectra the range is set from 0-25 keV, while **PIGE** spectra are shown from 0-2.0 MeV. These plot settings are one of the view setting that are not saved and will therefore revert to initial values whenever the program is started.

Options Menu



The Options Menu is called through **ctrl-o** and is used to set the names and parameters for external programs. **doiba** uses external programs such as **batty**, **thikc** and **thins** to extract peak areas from spectra and to calculate concentrations from these peak areas. These programs may be changed over time or different versions may exist for different purposes. This menu can be used to select a different version of the program to be executed.

The Standardfile is the data base containing information about the reference materials. With this parameter a different standard data base can be selected by the users.

In the section data conversion an external conversion program can be selected, that is called by the function **Convert Files**. This can be used to convert a foreign data format into the standard 9 column data format used

Figure 5: Option Menu.

2 EXTRA MENUS

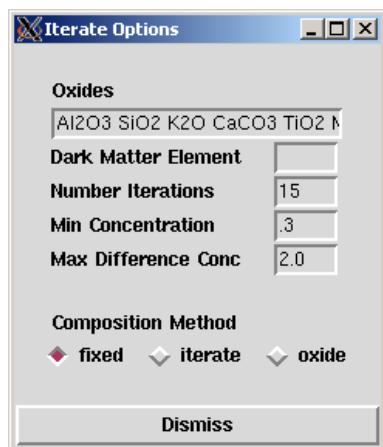
by **PIXAN** by calling an external program. The filenames for the data files must have the same structure as the **doiba** data files, except the extension. The file extension for the data files is given in the entry below.

The last section of the menu selects how the final results and especially results below the minimum detection limit (MDL) are reported in the output. Different ways of how results below the MDL are reported can be selected. Concentrations below MDL can either be reported as < mdl where mdl is the value of the minimum detection limit. Another option is to set the concentration to -99.99 when their value is below the mdl. This option may be selected when the data is further processed by another program that requires a numerical value. In a third option the concentration is reported as conc*, where the value is appended by a star (*), to mark that the result is below the mdl. The preferred option is < mdl, the other options have only been added in case the data is going to be used in other programs that require numeric values.

From the primary output file two Excel format csv files are derived, the first of these is a straight copy of the output file, which has a filename of the form **PROJECTNAMEXc.csv**. A second csv output file is created with the results rounded to the precision of the measurement. The number of significant digits for these results selected in the entry box **Decimal Places**. In this file results above 0.01% can also be selected to be reported in either percent or ppm, which is done with the radio buttons at the bottom of the menu.

Iterative

The Iterative Options Menu is called through ctrl-i and is used to control the behaviour of the iterative and oxide analysis methods.



Oxides

OXIDES

In **Oxides** an oxides form for each element can be defined. These are used to calculate the oxygen component in the matrix. For each element only one oxide form can exist. If more than one oxide form is given the last one appearing in the list will overwrite any oxide defined previously. As the list shows molecules such as CaCO3 can also be defined, as long as only one element in the molecule is part of the **PIXE** or **PIGE** output. In this case another bin for carbon is automatically opened in which the carbon component of the molecule is collected.

Figure 6: Iterative Options Menu.

Dark Matter Element

DARKMATTERELEMENT

Dark Matter Element is the element that is used to make up the remainder of the matrix missing for a total of 100%. Any element can be chosen as dark matter element, however, only oxygen or carbon should be used. If **Oxide** mode

is chosen, the **Dark Matter Element** field should be cleared. If the field it is not empty it will be used in a similar way as in the iterative mode, and the difference between calculated the matrix and 100% will be made up by the element in this field. The only difference is that, when the matrix is greater then 100% the value for the dark matter element can be negative, and it will be subtracted from the oxygen total. In this way the value for dark matter oxygen can be used as a measure of how consistent the results are.

Number Iterations

NumITERATION

Number Iterations defines the maximum number of iteration. When this number of iterations is reached the iterative process stops, regardless whether it has converged or not.

Min Concentration

MinConcITER

Min. Concentration is the minimum concentration an element has to have to be included in the list of matrix elements. All elements with concentrations smaller than this value will not be included in the matrix composition. This limits the number of elements in the matrix composition.

Max Difference Conc

MaxConcDiffITER

Max. Difference Conc is the largest relative change in the concentration of any element before the iteration stops. When the results for all elements change by less then this value the iterative process stops.

Composition Method

The **Composition Method** selects the method that is used to define the matrix composition for the samples.

3 Files

There are a number of files required to run the programs of the **doiba** package. These can be divided into Input, Run Control and Output files.

3.1 Input Files

The only input files to be provided by the user are the spectrum data files. Optionally a batchfile can be used to define the list of spectra to be analysed.

3 FILES

Name	Example	Format
PIXE Datafile	pixe001.rpt	rpt format
PIGE Datafile	pige001.rpt	rpt format

Table 1: List of input files used in the **doiba** package.

Program	Example	Comment
doiba	05feb08.Irc	doiba rc (output)
PIXE calibration	05feb08.Xcrc	PIXE rc
run batty	05feb08.Xbrc	PIXE rc (output)
batty rc file	05feb08.brc	batty input file
run conc	05feb08.Xrc	PIXE rc (output)
conc rc file	05feb08.crc	thin or thik input file
PIGE calibration	05feb08.Gcrc	PIGE rc (output)
run ptanal	05feb08.Grc	PIGE rc (output)
ptanal rc file	05feb08.ptrc	ptanal input file

Table 2: List of run control files used in the **doiba** package.

3.2 Run Control Files

There are a number of file that store the parameters for each step along the analysis chain, namely **Run Batty**, **Run Conc**, **Calibrate PIXE** and **Calibrate PIGE**. Additionally there are also the input files for the underlying programs such as **batty**, **thikc**, **thins** and **ptanal**. These files are generated automatically by **doiba** and they control the operation of the underlying programs. At this stage they are kept for debug purposes only. A list of all the run control files is shown in Tab. 2.

The table shows that the parameters for **PIXE** and **PIGE** are stored in different files. This has historical reasons, but this structure has been kept to be able to use **doiba**, **dopixe** or **dopige** on the same data set. All additional parameters not used in **dopixe** or **dopige** and common all common parameters are stored in the **doiba** rc. Newer versions of **doiba** also store a copy of the **dopixe** and **dopige** parameters, thus removing the need to load 3 different files to reload an old parameter set. If none of the parameters has been changed between the different analysis steps the **doiba** rc will contain the complete set of parameters of the analysis.

All the **doiba** run control files can be read by the program through **rc-Files**. This allows to read previously used parameter sets, and saves the need to type them in by hand.

3.3 Configuration and Data Files

There are a number of configuration files and data files that are used by **doiba** as well as the underlying **PIXAN** package. A list of them is shown in Tab. 3.

The **pige.config** and **filter.config** allow the configuration of the **doiba**. The **PIGE** part of **doiba** can be configured using **pige.config**. In this file the reactions that are used in **PIGE** can be changed and new ones defined. An example file adding a silicon reaction at 1.273 MeV is part of the **doiba** package.

filter.config is used to define the 3 predefined composite filters. These 2 files are either be placed in the **doiba** data directory or the users home directory. In the users home directory they have to be hidden files, which means the file names are preceded by a dot.

The **IBAPRINTER** and **beamlines** files are used to set the printers and beamline parameters. The **IBAPRINTER** contains a list printers on the system, while **beamlines** contains a description of beamlines and detectors. These can then directly be selected in the pull-down menus in **doiba**.

The **Standards** and **materials** are reference material and material data bases. The **Standards** file is required for calibration, while the **materials** file is used to easily select the composition of a number of materials from the data base rather than entering them by hand.

In the **ListOfCalibrations** file energy calibartions for a number of detectors can be stored. Double clicking on one of the energy calibration entry boxes brings up a selection box, from which a calibration can be selected.

3.4 Output Files

Output files can be divided into two categories, **doiba** output files and output files of the underlying programs such as **batty**, **thin**, **thick** and **ptanal**. Each spectrum is analysed individually by the underlying programs and a set of files is generated for each spectrum file. The names of these file have the structure **core###.ext**, where **core###** is identical to data file.

For **doiba** output files the **PROJECTNAME** forms the major part of the file name. These are the files the users will be most interested in. Most of the other files are only useful for debugging purposes and are therefore deleted when the **doiba** is closed down through the **Exit** command.

4 Executable Functions

In **doiba** the sample analysis is a multi-step process. The first step is to fit the experimental spectra and extract peak areas, while in the second step the peak areas are converted into concentrations. The first step is performed by **Run Batty** and the second by **Run Concs**. A 2 step process is used to allow the fitting of the spectra to be optimised first. This step may have to be performed a couple of times before the best fit to the data is found. The fit has to be optimised so that the fitted background

4 EXECUTABLE FUNCTIONS

Filename	Location	Function
Standards materials	doiba data directory doiba data directory	data base for reference materials composition data base for different materials
IBAPRINTER .ibaprinter	doiba data directory users home directory	list of printer names used by doiba same as above, overwrites the above
beamlines	doiba data directory	defines beamline and detector parameters to be selected by menu
ListOfCalibrations	doiba data directory	list of energy calibrations for different beamlines
filter.config .filter.config	doiba data directory users home directory	custom defined filters same as above, overwrites the above
pige.config .pige.config	doiba data directory users home directory	configuration of PIGE reactions used same as above, overwrites the above

Table 3: List of configuration files used by the **doiba** package.

Program	Example	Comment
Calibration	05feb08.calib	PIXE calibration output
batty	05feb08.area	batty areas
thin or thick	05feb08.conc	concentration output
oxide or iter	05feb08.comp	composition output
Calibration	05feb08.Gcalib	PIGE calibration output
ptanal	05feb08.Garea	PIGE area output
ptanal	05feb08.Gconc	PIGE concentration and area output
doiba	05feb08.pdf 05feb08Xa.csv 05feb08Xc.csv	pdf summary of analysis summary of PIXE areas in csv format summary PIXE and PIGE concentrations in csv format
	05feb08Ga.csv 05feb08XcR.csv	summary of PIGE areas in csv format summary PIXE and PIGE concentrations in csv format, rounded results
batty	pixe001.area	batty area output
batty	pixe001.plot	batty fitting output
batty	pixe001.bout	raw batty output
thin or thik	pixe001.conc	raw thin or thik output
doiba	pixe001.rps	postscript of fitting output
ptanal	pige001.ptarea	ptanal area output
ptanal	pige001.ptout	ptanal raw output
doiba	pige001.rps	postscript of ptanal fit

Table 4: List of output files created by the **doiba** package.

realistically represent the bremsstrahlung background in the spectrum, but also to capture all the elements present in the sample.

4.1 Run Batty

Run Batty starts the `batty` fitting procedure. The `doiba` package is intended for analysis of a large number of samples in a single step. There are two different ways to select the spectra files that will be analysed. The first is by selecting `use batch` in which case the `BATCHFILE` is read and all files listed in the batchfile will be analysed. Since the batchfile may contain a large number of files, which can take some time to fit, a second mode is provided. In this mode a range of files can be selected through the parameters `FIRSTNUMBER` to `LASTNUMBER`. This is useful to test and fine tune the fitting parameters for a smaller number of spectra. However, it may also be used to analyse a large number of files without the need to prepare a batchfile.

If `use batch` is selected the `BATCHFILE` is evaluated and all the spectra included in the batch file are fitted. Apart from selecting the spectra to be analysed the batchfile also allows to change selected parameters individually for each sample. In this case the `CHARGE:`, `COMP:`, `CARBON:` parameters in the batch file are evaluated and used to change these parameters individually for each sample.

During the analysis the output of `batty` is displayed in the message window. This can be used to trace and debug errors occurring in `batty`. `batty` is run using the control file `PROJECTNAME.brc`. For debug purposes this file can be used to run `batty` manually.

When the `batty` analysis is finished the results are summarised in the Report Window, an example of which is shown below (Fig. 7). The window shows a line with the peak areas for each samples. The first column gives the run number of the sample, which is the same number that appears in the file name. The third column is the sample name, which is taken from the `BATCHFILENAME`. If the program is not run in batch mode, it tries to read the sample name from the spectrum file. If no name is given in the spectrum file this entry will be blank.

From the report window the fitting procedure can be checked by clicking **Show Spectra**. At this stage it should be checked if the background is fitted correctly and if all the peaks in the spectrum have been fitted. In case some of the peak have been missed additional elements have to be added into the list of `ELEMENTS`.

When this step is completed and all the spectra have been fitted satisfactory, the extracted areas can be converted into concentrations using **Run Concs**.

When **PIGE** analysis is selected the peak areas for **PIGE** are extracted simultaneously using `ptanal`. Therefore it is advisable to leave **PIGE** switched off while testing the **PIXE** fitting and only use this option in the final fitting run. Once `ptanal` is finished the results are summarised in the **PIGE** Report Window (see Fig.8). This output has the same format as the `batty` output.

Fig. 9 shows a typical fit of a **PIXE** spectrum with `batty`. The figure shows three different graphs. The black graph is the original spectrum, showing a large number of characteristic X-ray lines between 1 and 20 keV. The red line shows the background

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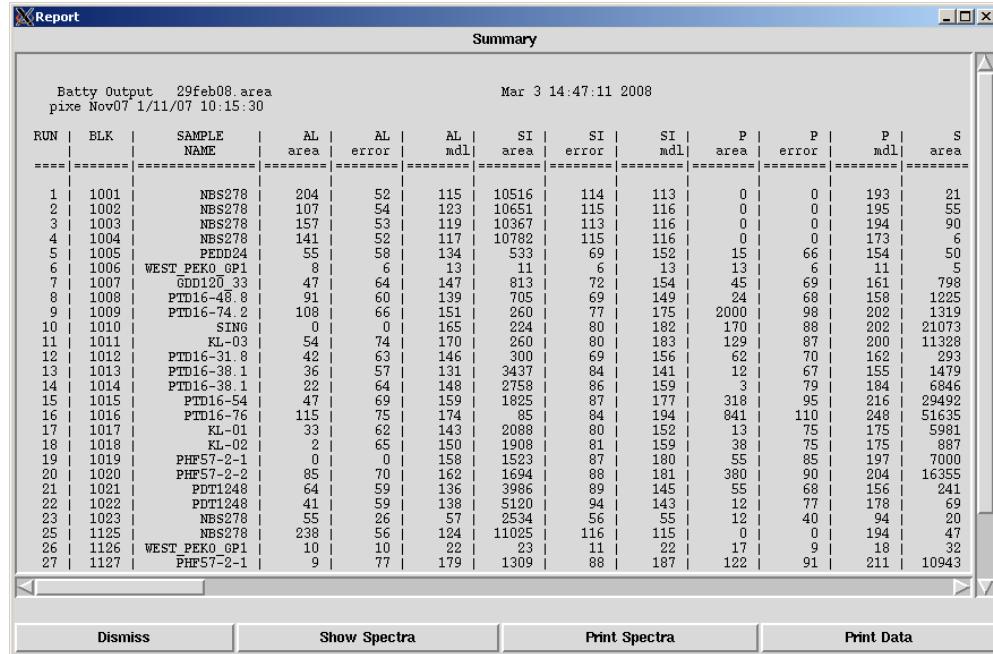


Figure 7: **batty** output summarised in the Report Window.

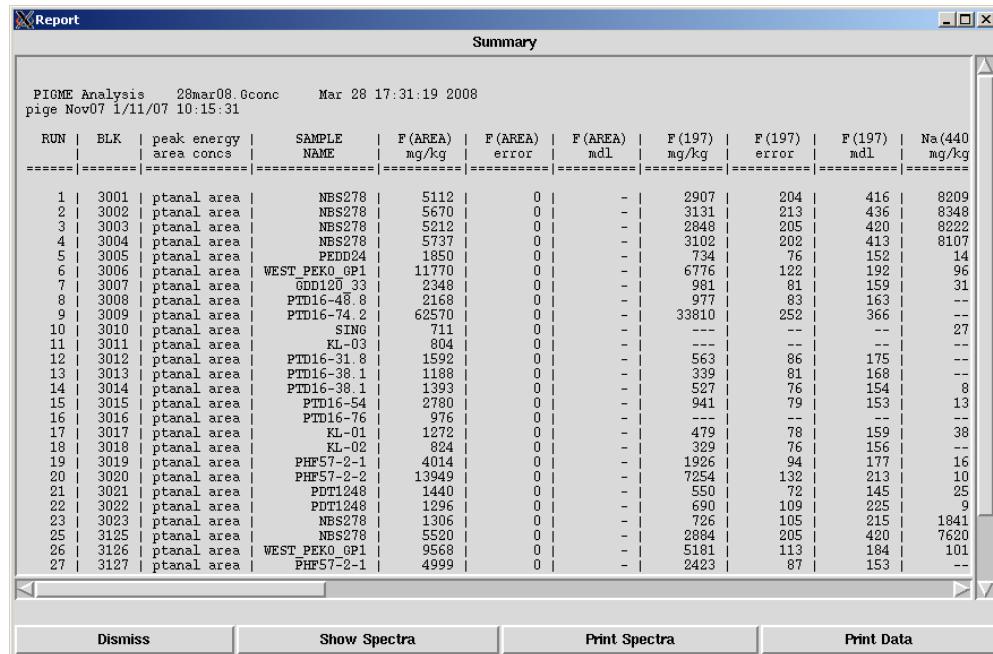


Figure 8: **ptanal** output summarised in the Report Window.

4.1 Run Batty

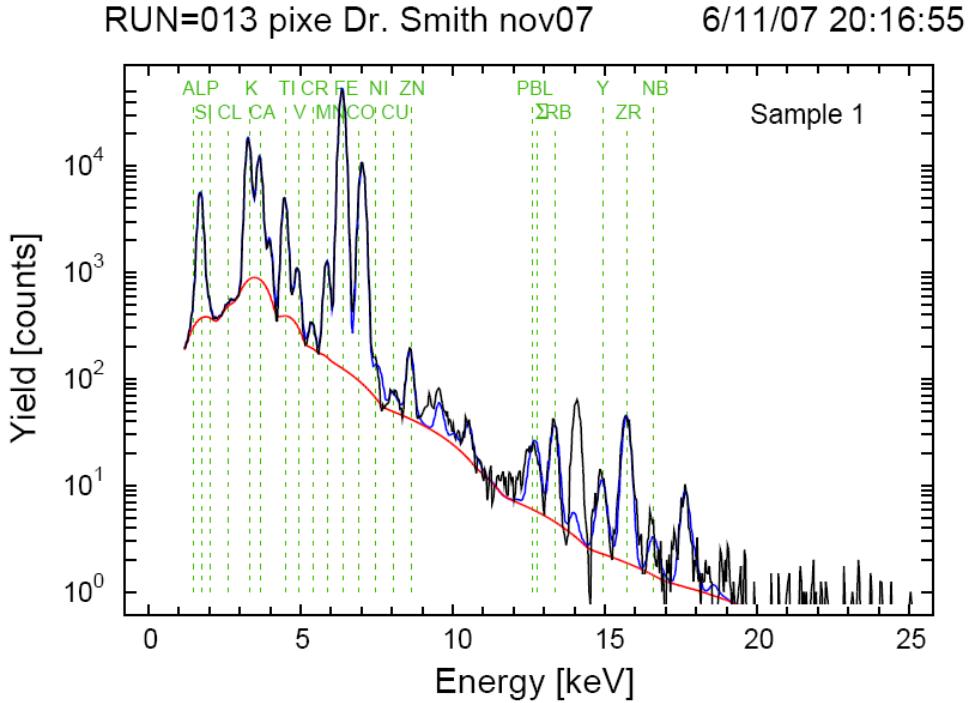


Figure 9: **batty** fitting of **PIXE** spectrum with batty. The peak at 14.1 keV not fitted in the spectrum means an element, in this case Sr is missing in the list of **ELEMENTS**.

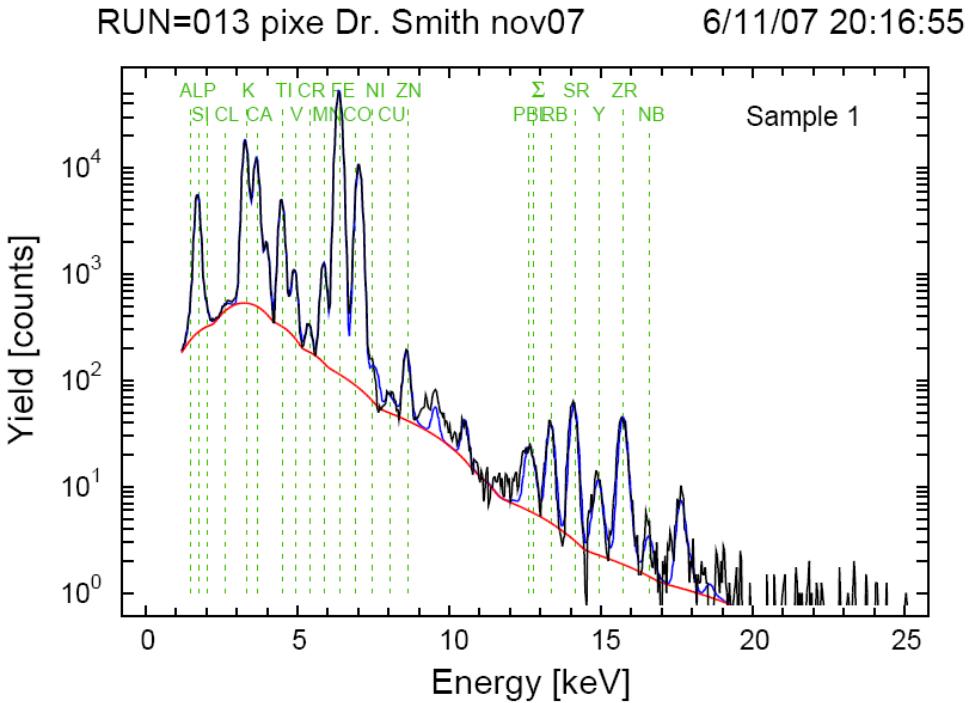


Figure 10: A better fit of the spectrum by **batty**. This time all peaks are fitted. The background also better represents the bremsstrahlung background.

4 EXECUTABLE FUNCTIONS

subtracted from the spectrum by `batty`, while the blue line show the total fit, with the green markers indicating the elements found by `batty`. The figure shows a very good agreement between the fit and the spectrum. However, a characteristic X-ray line at 14.1 keV has not been fitted, indicating Sr in the sample. A closer inspection also shows that the background is bulging to far into the X-ray peaks. This is because the value for the curvature in the background fitting is too large.

After adding Sr to the element list and changing the value for the `CURV` from 1.002 to 1.0005 the fit is repeated, resulting in graphs of Fig.10. [6] The graph shows that now the peak at 14.1 keV has been fitted and the fit for the bremsstrahlung background is more realistic.

4.2 Run Concs

Run Concs calculates concentrations from the peak areas extracted before by `batty`. The behaviour of **Run Concs** changes depending on whether the **PIGE** analysis is turned on or off, thin or thick targets are selected and most importantly if an iterative calculation of the matrix composition is selected.

When **PIGE** analysis is turned on both **PIXE** and **PIGE** concentrations are calculated and the results are combined in a single output file. Otherwise only **PIXE** concentrations are calculated.

For thick sample in both **PIXE** and **PIGE** the stopping of the ion beam in the target material is taken into account, while for **PIXE** the self-absorption of the X-rays is included as well. In order to account for both the composition has to be known, before the calculation. Although in principle the composition can be determined from the two measurements, this is not straight forward since not all elements can be measured. Hence a number of different ways can be selected in the analysis software to estimate the composition.

The simplest approach is to require the matrix composition to be given as an input in order to calculate concentrations. This seems like a contradiction for an analysis: the need provide the composition in order to get the concentration of elements. However, in a number of cases the matrix composition is fairly well known and moreover small changes of the composition only change the results within the margin of error. This is the case in a large number analysis undertaken in our laboratory, where know materials like obsidian are analysed for trace elements.

On the other hand, it would be useful to have a way to extract concentrations without the need to provide a matrix composition. Fortunately this can be done by making a few simple assumptions about the samples. Firstly the elements than can not be detected by either **PIXE** and **PIGE** are generally elements lighter then fluorine. In most samples this would probably be oxygen from an oxide formed with some of the heavier elements in the sample. It can be assumed, that in most cases the missing fraction to make 100 % is mainly oxygen. An iterative procedure can then be used to calculate the matrix using the **PIXE** and **PIGE** results. To allow for more flexibility the element used to complement the matrix can be set by the user.

However, if the oxygen in deed comes from an oxide formed with one of the heavier

elements the oxygen content can be calculated directly. Hence, in a second method a oxide form can be specified for each element, which is then used to calculate the total amount of oxygen. In this case the dark matter element has to be blank. If oxygen is given as a dark matter element it will behave very similar to the iterative approach. If the total matrix including the oxygen from the oxides is smaller or larger then 100% the difference is made up by the dark matter oxygen. When the total matrix is larger then 100% the dark matter oxygen will negative. In this way the dark matter element is used to adjust the total matrix to 100%.

On the other hand if the field for the dark matter element is left blank, the total matrix is adjusted by expanding it to 100%, while keeping the elemental ratios the same.

For both iterative methods the field for the matrix composition has to be left blank. Any elemental concentration given in the composition field will be added to the calculated concentrations. This can be useful if the samples have been mixed with a known amount of graphite or some other material. In this case this amount is added to the calculated composition and will not be varied.

4.3 Calibrate PIXE

The **Calibrate PIXE** function allows the calibration of the **PIXE** analysis. The name of this function is somewhat misleading, because **PIXE** does not need calibrating and indeed cannot be calibrated. However, a number of **PIXE** parameter may change slightly from experiment to experiment and need to be adjusted and checked. This function provides an interface to do both in a convenient way using a standard reference material.

Parameters that may have to be adjusted are the filter parameters, distance of detector, Be window thickness, ice thickness and total charge. Figure 11 shows the calibration window, which contains all these parameters in a single window. When the function is executed the program calculates the concentrations for all the samples in standard string and compares them with the standard value given in standard data base.

The Calibrate **PIXE** window has a number of function buttons that help to refine the parameters. These functions are Summary, last Calib, Plot Calib, Plot Size, Auto Calib, QA DataBase, Run Again, x-ray Yield and Plot Size.

The lower part of the Calibrate **PIXE** window summarises the analysis results of the standards. Comparison with the certified reference values can then be used to improve the analysis parameters. Above the results window is a list of all the elements in the standards with a tick box next to the name. In the standard data base a reference value can be marked as certified. If a value is marked as certified this box will be ticked for this element. This method is ambiguous, when different standards are used, since the values for one element may be certified in one standard, but not in one of the others. Hence it is advisable to use one reference material at a time.

To help optimise the parameters the ratio of measured to standard value can be plotted for each element. This is done by the Plot Calib function and an example of a graph is shown in Fig 12. In this plot only the selected elements will be show.

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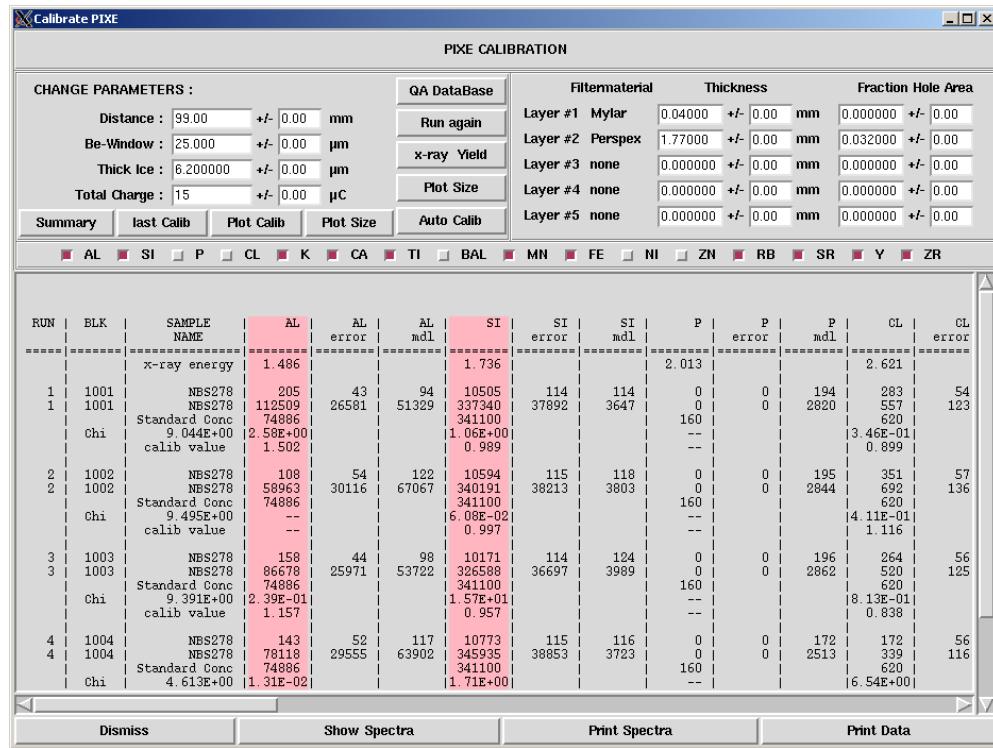


Figure 11: PIXE Calibration Window.

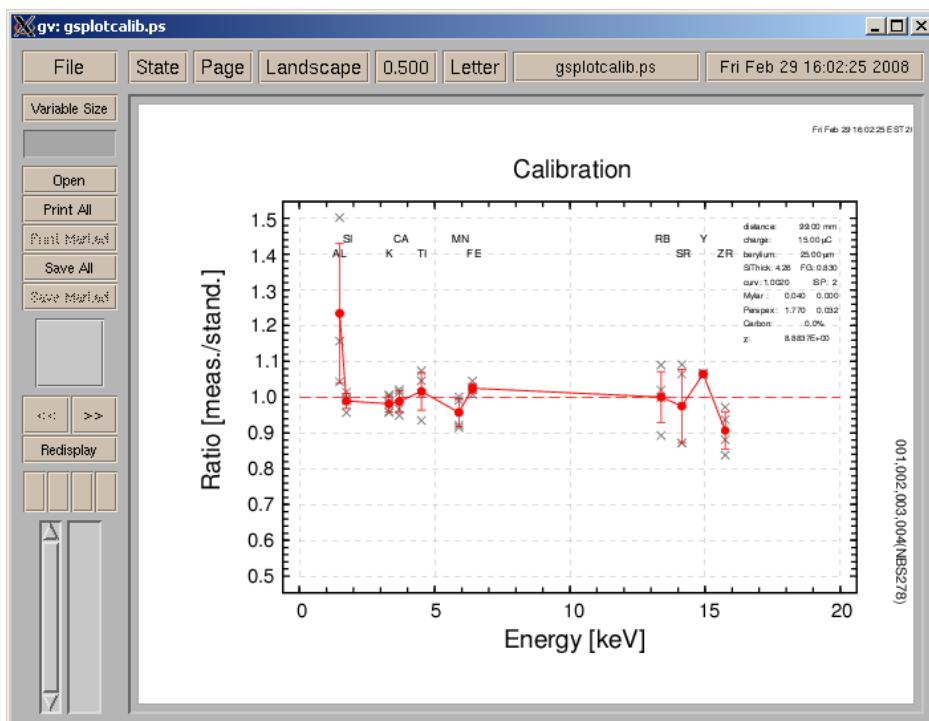


Figure 12: Plot of PIXE calibration results.

4.4 Calibrate PIGE

In this way elements for which the concentration is not certified or not well known can be suppressed. The results for each individual standard are indicated by a gray x, while the average and the standard deviation are marked by red dots and error bars. The results for each individual standard are shown, to help identify if one of the measurements is systematically different.

The graph also helps to decide which parameters have to be changed in order to improve agreement between measurement and certified values. When all the measured values are either too small or too large by the same fraction, this is a strong indication that either the charge or the detector distance have to be adjusted. Changing either of them will shift the whole graph up or down. In fact in this case it is difficult to decide which of the two parameters should be changed.

If a discrepancy only exists for Al and Si, then measurement can be improved by changing the Be-window thickness. The plot Calib window also allows to track these changes and monitor the agreement between measured and certified values. In order to do this the Run again function has to be used. When the analysis is rerun using Run again, the results of the previous analysis are kept and plotted together with the new results. The Run again function can be used repeatativly and a number of times, however, the graph becomes crowded when too many results are shown on top of each other. The calibration can be reset by running the calibration from the main menu through Calibrate **PIXE**.

The graph can be resized using the Size Plot function. However, in order to view the resized graph the function Plot Calib has to be called again. When the function Run again is used the new results will be appended in the result window. The last Calib function, deletes all previous results and displays only the results with the actual parameters, while Summary produces a summary of all calibration analysis runs.

The Auto Calib and QA DataBase functions can be used to call external programs that automatically optimse the parameters to achieve good agreement between measured and certified values and display and manage a data base of previous values of the parameters. The DataBase function is useful to monitor parameters that will change over time such as the ice thickness. Both functions require external programs, which are not available on all systems.

For the **PIXE** calibration parameters a range can be defined, which is used by the X-ray Yield function. This function visualizes the change of the X-ray yield for variations of the parameters. The output graph can be resized using the Plot Size function directly underneath the X-ray Yield button.

4.4 Calibrate PIGE

PIGE is a calibration technique and a standard is required. After the Calibrate **PIGE** is pressed the **PIGE** Calibration window Fig 13 opens. This window displays the major parameters of **PIGE**. It allows the user to adjust these parameters and try different values during calibration. However, these parameters only influence the way the **ptanal** will find and identify peaks in the spectrum.

This menu also has 6 buttons, Exit, Plot Calib, Print Calib Plot, Scale Calib,

4 EXECUTABLE FUNCTIONS

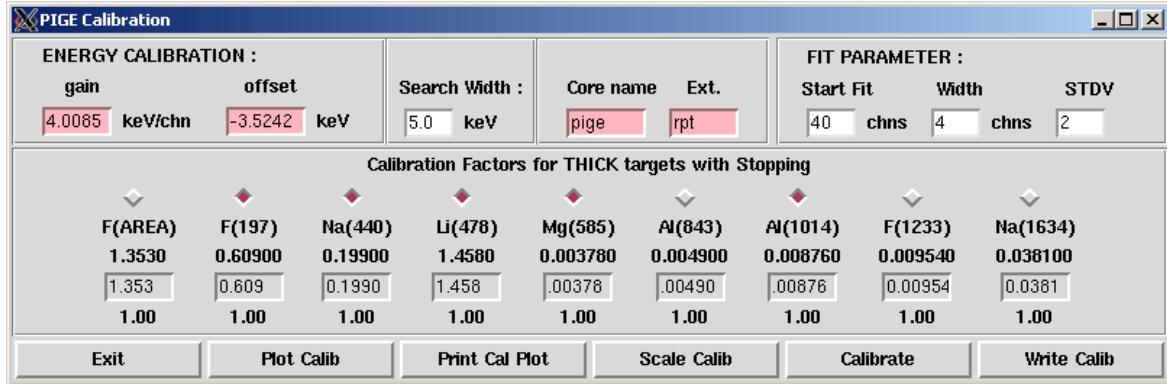


Figure 13: PIGE calibration window.

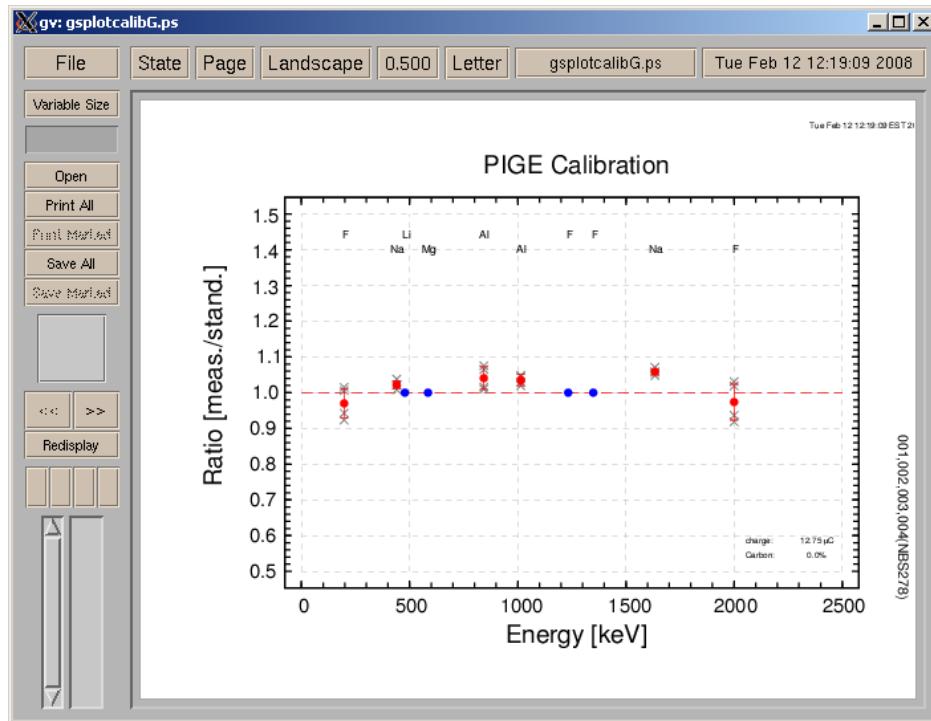


Figure 14: PIGE calibration window.

Calibrate and Write Calib. Exit is used to exit and close the **PIGE** Calibration window. Calibrate executes the **PIGE** calibration. In this case the peak areas for the γ peaks are calculated and compared with the concentration of the respective element in the standard. As in the **PIXE** calibration only the samples that are listed in the standard list are analysed. As a result for each reaction a new calibration value is calculated and displayed in the entry box. Above the entry box the original calibration value is shown, while the value below the box shows the ratio between the original value and

the new value.

Plot Calib will show the ratios for the new calibration value versus the original calibration value, for all the **PIGE** reaction. This graph can help to reveal systematic errors. In case the standard is mixed with some amount of graphite and this has not been taken into account there will be constant shift for all reactions. The same will apply for any systematic errors in the charge measurement. In this way this graph can help to identify some simple mistakes that can appear.

A long term average should be used as original calibration value. At this stage the experimental geometry as well as the detector parameters are not taken into account, therefore the calibration values depend on the experimental setup and the long term averages have to be determined separately for each experimental setup.

With Print Calib Plot this calibration will be printed on the printer selected in the main menu, while Scale Plot allows to re-scale the x and y axis of the graph. Write Calib will write the calibration to the file `pige.calib` in the current working directory. This file is read the next time when `doiba` is started, thus allowing the user to access the previous calibration. However, whenever a calibration is performed this file is automatically written and there is no need to write the file manually.

On the other hand calibration values can be entered manually. This may be done in cases where a standard does not result in a good calibration for some elements. In this case the user can enter his own calibration values for these elements in the entry box. These values will then be used in any subsequent analysis, however, they will not be saved automatically. This means they will not be available the next time `doiba` is run, unless they have been saved manually using Write Calib. Therefore it is recommended, whenever a calibration value is changed by hand to execute Write Calib.

The **PIGE** Calibration menu is also used to select the reaction, that is used in the iterative and oxide modes. In both modes the matrix composition is calculated from the **PIXE** and **PIGE** results. For some elements a number of γ -rays can be used to calculate their concentration. For Al for instance p- γ reactions with γ -ray energies of 0.843 MeV and 1.014 MeV can be used. To select which reaction should be used the tick-box above the reaction has to be selected. For each element only one reaction can be selected.

Some elements, such as Al, Mg and Na can also be measured with **PIXE** and in the iterative and oxide mode the **PIXE** analysis is always selected over **PIGE**. In order to use the **PIGE** analysis for these elements they have to be removed from the shopping list before calculating the concentrations. In order to achieve a better fit of the **PIXE** spectra these elements should remain in the shopping list during the fitting procedure.

4.5 Exit

The **Exit** function closes down `doiba`. There are different options that can be selected before the program shuts down. The Exit Window is shown in Fig. 15. `doiba` creates a number of temporary files, some of them can be used for debug purposes and can be consulted to improve the analysis. By and large they will not be needed any longer

5 COMMAND LINE OPTIONS

after the analysis is finalised. By selecting clean up in the Exit Window, these files will be deleted.

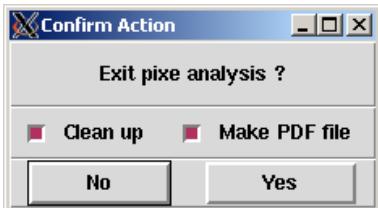


Figure 15: Exit Window.

After closing [doiba](#) a pdf document can be created. This document is intended as a summarising report of the analysis and contains all the data of the analysis, such as a table with all the concentrations, but also all the **PIXE** and **PIGE** spectra. This documents is intended to be sent to the customer.

Additionaly the results of the calibration procedure, such as a table with the calibration results as well as the graph of calibration can be included. If the calibration results are not be included in this document, this can be de-selected in options menu.

5 Command Line Options

[doiba](#) has a number of command line parameters that can be used to include the program in scripts and produce simple programs to analyse a number of data set using predetermined parameters. A list of command line options is given by

```
doiba -?
```

which is shown in the listing below. Most of the command line options are used to read configuration files. The **-c** and **-config** options are used to read **thick**, **thin** and **batty** config files. These options were original included to read historical run control files from these programs.

The **-Iconfig**, **-Xconfig** and **-Gconfig** are used to load the [doiba](#) run control files. These files can be appended by a number of commands, which will be executed after the file has been read. The commands are shown in the listing below. Most of them are equivalent to the Executable Functions in section 4. These commands can be mixed with Unix commands. In this way an interface is available to write scripts to analyse a number of different data sets. Since the commands and parameters are read sequentially, the order of the commands is important.

doiba command line options

doiba	version 0.90	29. Oktober 2007
	IBA Analysis	
-f filename	filename with parameters for standards	
-c filename	filename of brc and crc files, without extension	
--batch filename	filename of batch file	
--config filename	filename of brc and crc files, without extension	
--Iconfig filename	filename of IBA rc file, with extension	
--Xconfig filename	filename of PIXE rc file, with extension	
--Gconfig filename	filename of PIGE rc file, with extension	
--auto filename	run batty & conc automatically using doPIXE rc file	
-nofix	stops the fix of the calib problem in batty	
-fix	use the fix of the calib problem in batty	
-?	this help	
--help	this help	

```
The following commands can be used in the Iconfig file
each command has to be on a separate line
```

```
Exec unix-command
cd directory
RunBatty PrintBatty
RunConc PrintConc
RunCalib PrintCalib PlotCalib

RunPTANAL PrintPTANAL
RunGCalib PrintGCalib PlotGCalib
Exit
```

The behaviour of RunCalib and RunGCalib, is slightly different from the behaviour of their equivalent in the GUI interface. Both commands execute an EvaluateBatchfile command, which means the batchfile, if it exists, is searched for Reference Materials listed in the Standard database. Any sample name that appears in the standard database is included in the list of standards and analysed in the calibration. To bypass this behaviour, the **BATCHFILENAME** has to be cleared, before RunCalib is executed. However, the batchfile can be set afterwards to be used in the analysis. An examples of how this can be done is shown below.

Example of the use of **doiba** functions in the **rc** file

```
#  
# first set IBA parameters  
#  
[IBARC]  
BEAMLINE: SR2  
PIXEPATH: pixe  
PIXEINFILENAME: pixe  
BATCHFILEON: 1  
BEAMENERGY: 2.50000  
CompELEMENTS: NA AL SI CA K FE O  
ConcELEMENTS: 3.23 6.79 34.30 0.89 3.63 1.78 39.14  
. .  
PIGEANALYSISON: 0  
#  
# next set the parameters for PIXE  
#  
[PIXERC]  
ENERGYSLOPE: 0.019900  
ENERGYOFFSET: -0.050000  
DXBE: 25.000  
DXSI: 0.3000  
DXAU: 0.0200  
DTHIK: 4.2600  
.
```

6 ADDITIONAL COMMAND LINE TOOLS

```
.  
#  
# set a projectname to overwrite the one generated  
#  
NEWPROJECTNAME: AUTORUN  
#  
# make sure the batch file name is empty before calibration  
# and then define the standards to be used in calibration  
#  
BATCHFILENAME:  
STANDARDSTRING: 7,106(NBS278)  
RunCalib  
RunGCalib  
#  
# after the calibration is done set batch file name  
# for analysis RunBatty and RunConcs  
#  
BATCHFILENAME: 20nov07.batch  
RunBatty  
RunConcs
```

The file should set the values of all parameters in the first part. Although *PROJECTNAME* is saved in the run control files it is not set when the file is read. This is to avoid using the same name for all subsequent analysis. However, in order to be able to set this variable the identifier *NEWPROJECTNAME* is available. The above example thus first clears the *BATCHFILENAME*, then defines the files containing the spectra with the NBS278 standard to be number 7 and 106 and then executes the calibration. After that the *BATCHFILENAME* is set to be used in the *batty* and *concs* analysis.

6 Additional Command Line Tools

The **doiba** package comes with a number of tools to provide assistance prior to or after the analysis. Some of these tool have a graphical user interface, while other are simple command line tools. Tools having a GUI are generally linked into the **doiba** program itself and can be called from **doiba** gui. However, they can also be used as stand alone programmes.

6.1 File Viewer

The File Viewer is called by **fv**. Fig. 16 shows the interface displaying an **batty** plot output file. The File Viewer is intended for quickly viewing text or data files. It recognises the spectrum and batty plot output format and automatically plots these files as graphs rather showing them as ASCII text. All other files will be displayed

as ASCII text. It can be accessed in [doiba](#) through the File Viewer button at the bottom.

[fv](#) command line options

```
fv           version 0.6      12. July 2007
File Viewer  [-p pattern] [files]

-p pattern    pattern for files
              don't forget put pattern in inverted commas
-?            this help
--help        this help
```

6.2 Batch Editor

The [batch-editor](#) can be used to create and easily edit batch files. Fig. 17 shows the batch-editor interface. On the right side is it has sections for materials, carbon and charge. In each of these sections is a listbox with a number of selections. Double click on a material from the materials list and the selection will be inserted as composition for the current sample, marked by the red line. If the sample already had a composition next to its name this will be replaced by the selected one. The charge and carbon content fields work in the same way.

6.3 Extract Batch Tool

Another way to create a batch file is the tool [extract-batch](#), which automatically creates a batchfile including all data files in the directory, where [extract-batch](#) is executed. It is searching for all files with the same extension and will extract the sample name. It then creates a file with the file numbers and sample names in the batchfile format. The extension of the data files can be set by the command line option -e. Other command line options of [extract-batch](#) are shown below.

[extract-batch](#) command line options

```
extract-batch          version 0.9          01. May 2002

Create batchfile from spectra

This requires the sample name to be recorded in the spectrum files

-f      filename name of batchfile to be created
-e      ext of data files to be searched
-?      this help
--help  this help
```

6.4 Standard Data Base Tool

The standard data base tool is a tool to extract the composition of a reference material from the data base. The command line options are shown in the listing below.

6 ADDITIONAL COMMAND LINE TOOLS

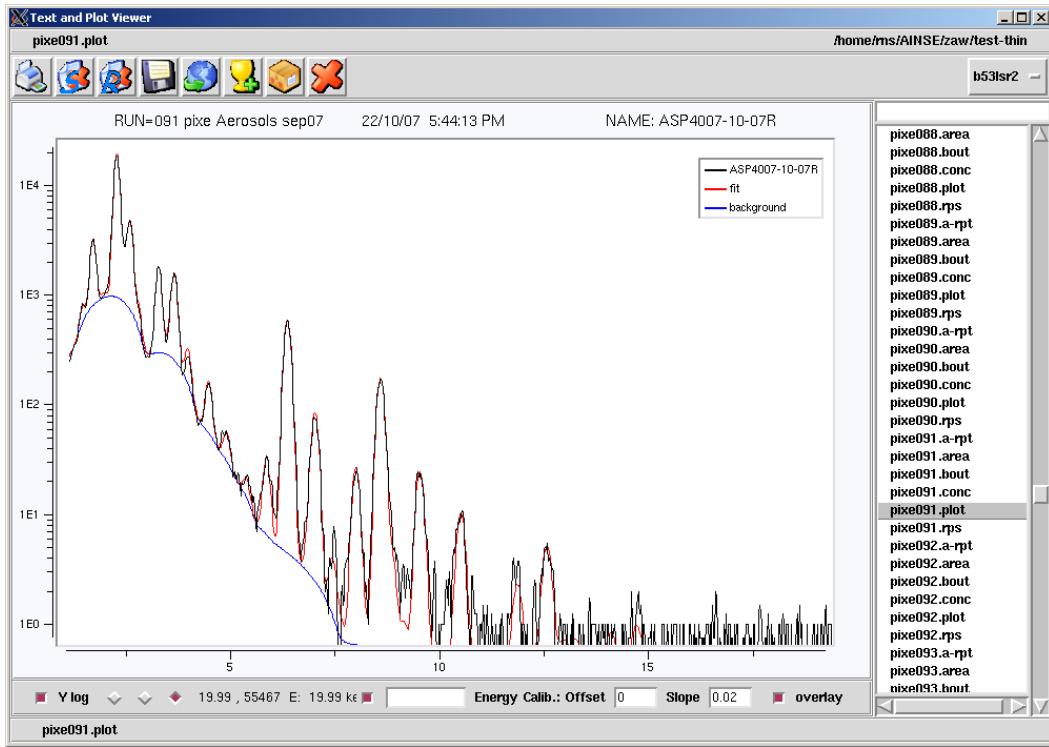


Figure 16: `fv` interface.

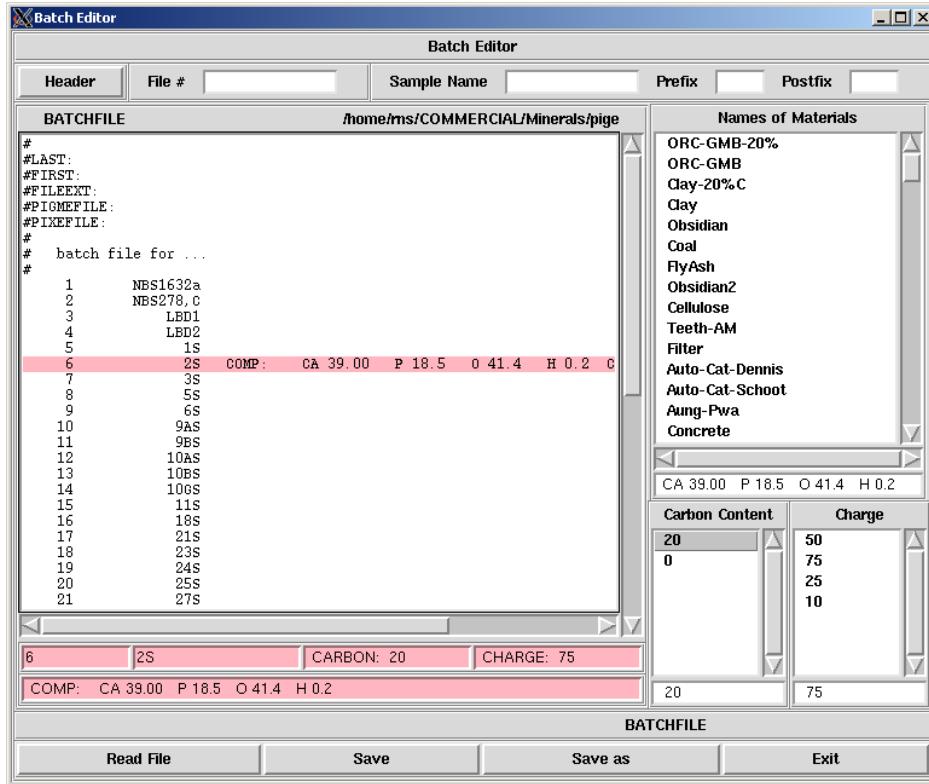


Figure 17: `batch-editor` interface.

standard command line options

```
standard shell script to extract reference material composition from
/usr/local/pixan/data/Standards

usage standard [LIST] standardname.

[-?] this help
```

Running **standard** without options will display a list of reference materials in the data base. With the name of a reference material as option it will display the composition and certified values of the material. An example for the usage of the program and its output are shown below.

Example of usage of **standard**.

```
boson:~$ standard NBS278
NBS278
O 48.88 %
LI 0 ppm
F 500 ppm
NA 3.59 %
MG 1387 ppm
AL 7.49 %
SI 34.11 %
K 3.45 %
CA 0.70 %
TI 1500 ppm
MN 403 ppm
FE 1.43 %
*NI 0 ppm
*P 160 ppm
BA 1140 ppm
*CL 620 ppm
RB 127 ppm
SR 64 ppm
ZN 55 ppm
ZR 290 ppm
Y 39 ppm
```

6.5 Periodic Table

doperiod a tool that displays the periodic table is provided to easily access the characteristic X-ray energies for elements. Clicking the right mouse button shows a list of X-ray energies, similar to **doiba**. It shows the characteristic energies together with the relative intensity of the line. For elements heavier then Sr both K and L-line energies are displayed, while for elements above Hf only the L and M-line energies are shown. The data from the dset2 data is used for the display and therefore if this dataset is changed this will change.

Clicking the left mouse button will display the physical properties of the element. Fig. 18 shows the **doperiod** window. The window shows as an example the display of physical properties. It shows the nuclear charge, mass and natural mass as well as the density and atomic density.

6 ADDITIONAL COMMAND LINE TOOLS

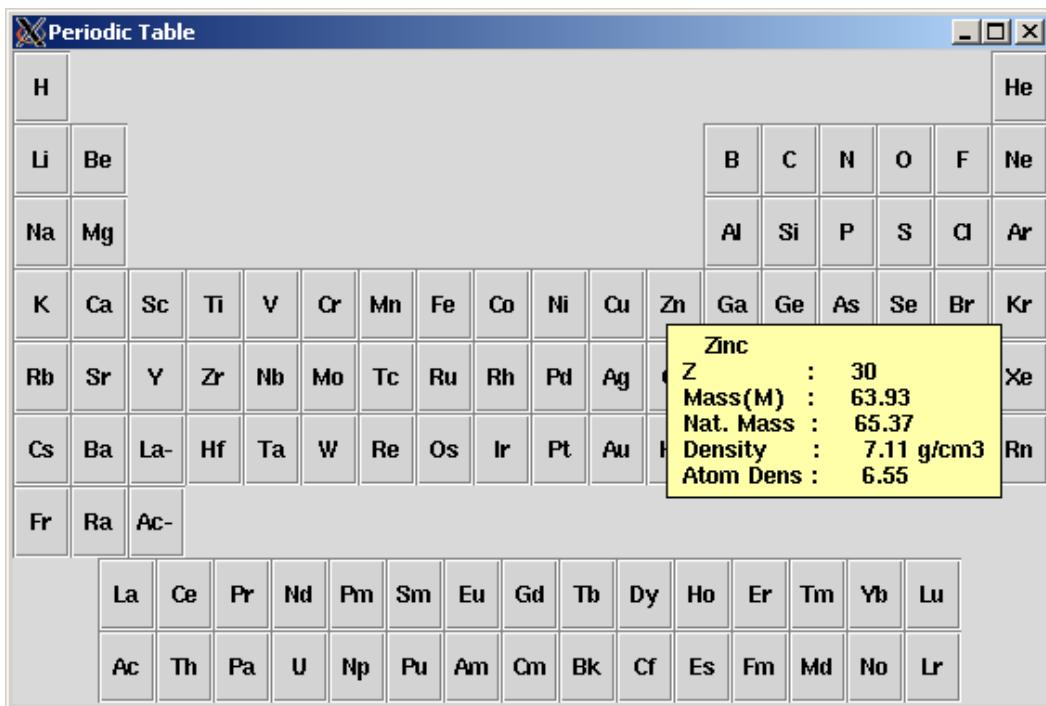


Figure 18: Main window of `doperiod` showing the display of physical properties for Zn.

6.6 Chemical Composition

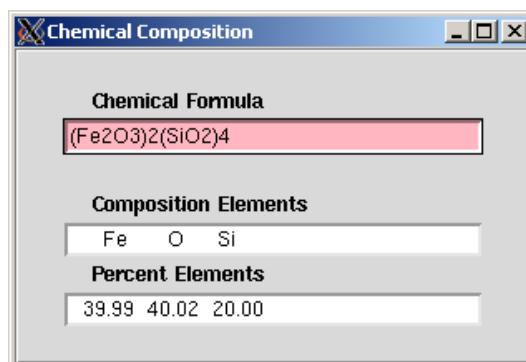
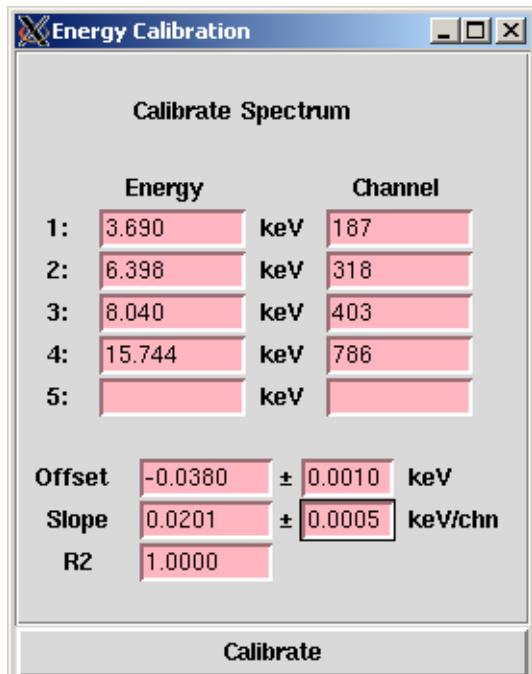


Figure 19: `dochemistry` window.

A tool to calculate elemental concentrations using a chemical formula is provided in `dochemistry`. Placing the cursor and in the entry box and pressing enter will calculate the concentration of the elements in weight percent, which is the input required by `doiba`. Fig. 19 shows the display of the program. The figure also gives an example what type of expressions can be used. Simple chemical formulas such as SiO2 can be used, but also more complicated formulas such as (Fe2O3)2(SiO2)4 can be entered.

The type of formulas is limited to single brackets, which means brackets can not be placed inside brackets.

6.7 Energy Calibration



An energy calibrations tool is provided to easily calculate energy calibrations for **PIXE** and **PIXE**. Fig. 20 shows the `docalib` interface. In the interface up to 5 energy channel value pairs can be entered. Using the calibrate button at the bottom of the window calculates the energy calibration using linear regression.

Figure 20: `docalib` window.

6 ADDITIONAL COMMAND LINE TOOLS

II Examples

7 Thick Sample Analysis

This section goes through the various steps of a normal analysis. It also compares results for the two different methods that can be used to calculate the sample matrix, which are the iterative and oxide method. In the examples we will describe a combined **PIXE** and **PIGE** analysis.

After all the parameters have been entered the first step is to run **Calibrate PIXE**. **PIXE** is a calibration free technique and the term calibrate **PIXE** is a somewhat misleading. What this step really does is verify some experimental parameters using a Standard Reference Material. It may also be used to tweak some parameters to get a better agreement between the measured and the reference values. For this purpose the **Calibrate PIXE** interface allows to easily vary these parameters and see how the ratio of measured to reference values changes for various elements.

We will also show how to use the different analysis modes. For this purpose the well known Standard Reference Material NBS278 was analysed. The example will also demonstrate the use of a composite pin hole filter, made of Perspex covered with mylar. The Perspex was measured to be 1.84 mm thick Perspex filter with a 0.75 mm diameter hole drilled into it. This is equivalent to 3.5% of the detector area (detector diameter is 4 mm). The hole is covered with a 40 μm thick mylar foil.

The parameters for this filter have been stored under the name Old-PinHole and are loaded by clicking the check-box. Running **Calibrate PIXE** will analyse the spectra listed as standards. For thick samples the composition stored in the standard database is used as sample matrix in the analysis. After the analysis is completed the **PIXE** Calibration window will (see Fig. 12) pops up, summarising the results.

The graphical representation of the calibration can be displayed through **Plot Calib**. The window shown in Fig. 21 will pop up displaying the calibration plot. Only elements selected in the Calibration window (see Fig. 11) will be shown in the calibration plot. This is useful to exclude elements for which the reference values are not reliable.

The graph shows quite a significant difference between the measured values and reference values for a number of elements. The shape of the deviation for light elements shows that the mylar foil must be thinner than the 47 μm . Reducing the mylar foil thickness to 45 μm and running the calibration again results in the blue curve in Fig. 22. However, there is still some difference for all elements up to Zn. Adjusting the thickness and the hole area, finally leads to the red curve in Fig. 22, which shows a good agreement between the measured and reference values of the standard. Y and Sr still show large deviation, but also have a large error. This is because these elements are present in very low concentrations.

The next step is the **PIGE** calibration. In contrast to **PIXE**, **PIGE** is a calibration

7 THICK SAMPLE ANALYSIS

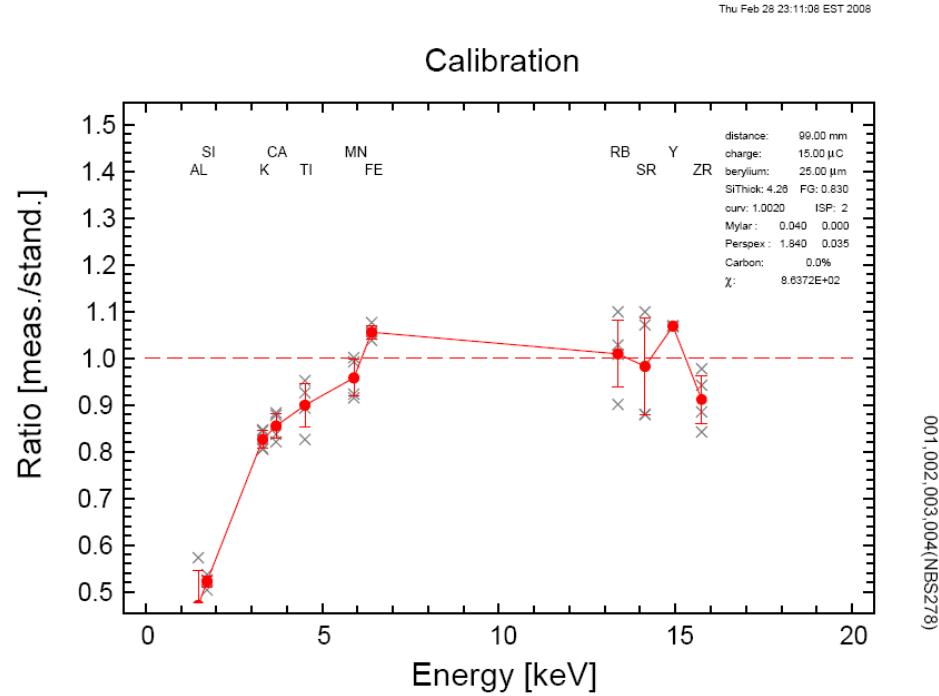


Figure 21: **PIXE** calibration plot. The plot shows that for light elements, the results are generally too low.

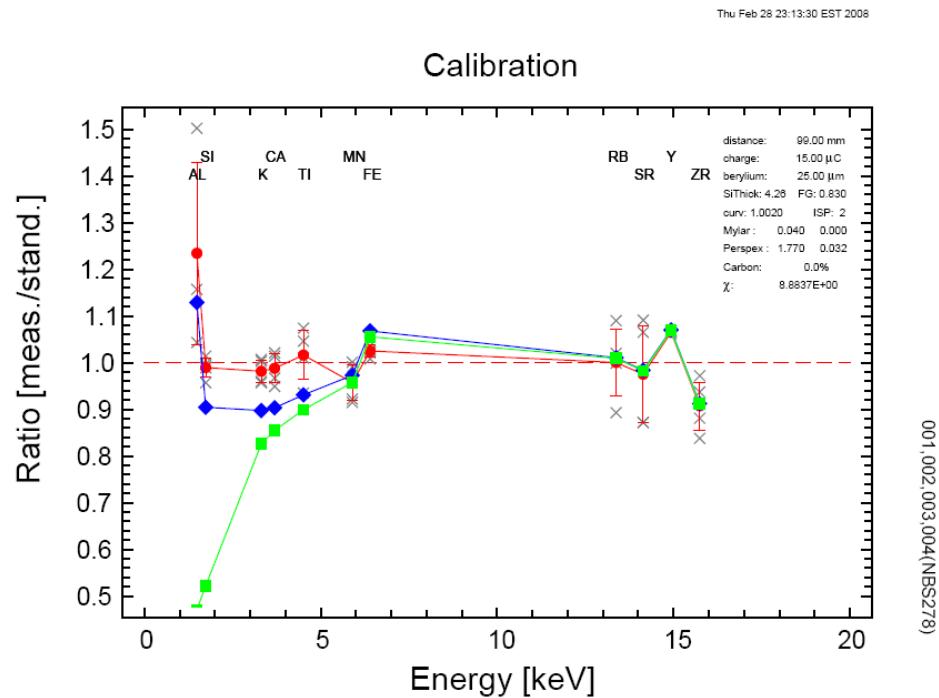


Figure 22: **PIXE** calibration plot, showing the results for various parameter sets..

SAMPLE	F(AREA)F	Na	Al	Si	K	CA	TI	MN	FE	ZN	RB	SR	Y	ZR	
NBS278	470	490	3.60%	7.4%	33.0%	3.2%	0.65%	0.16%	380	1.40%	41	120	65	43	240
NBS278	520	520	3.60%	7.4%	34.0%	3.4%	0.70%	0.16%	370	1.50%	45	130	67	43	280
NBS278	480	480	3.60%	7.6%	33.0%	3.2%	0.66%	0.16%	400	1.40%	51	110	56	42	270
NBS278	530	520	3.50%	7.6%	34.0%	3.4%	0.71%	0.17%	400	1.50%	49	120	56	< 35	260
NBS278	540	550	3.60%	7.5%	36.0%	3.8%	0.77%	0.17%	370	1.60%	61	130	78	< 82	270
NBS278	510	480	3.30%	7.4%	35.0%	3.5%	0.71%	0.16%	380	1.50%	52	110	61	32	230
NBS278	490	510	3.50%	7.4%	36.0%	3.5%	0.72%	0.17%	410	1.50%	44	110	70	46	280
Average	506	507	3.53%	7.47%	34.43%	3.43%	0.70%	0.16%	387	1.49%	49	119	65	41	261
stdev	5.2%	5.1%	3.2%	1.3%	3.7%	6.0%	5.7%	3.3%	4.1%	4.6%	13.5%	7.6%	12.2%	13.0%	7.5%
Certified	500	500	3.59%	7.49%	34.11%	3.45%	0.70%	0.15%	403	1.43%	55	127	64	39	290

Table 5: Results using oxide calculation, where the total matrix is complemented with oxygen through the oxide from of the element.

SAMPLE	F(AREA)F	Na	Al	Si	K	CA	TI	MN	FE	ZN	RB	SR	Y	ZR	
NBS278	470	480	3.60%	7.4%	33.0%	3.3%	0.66%	0.16%	380	1.40%	41	120	65	43	240
NBS278	520	520	3.60%	7.4%	34.0%	3.5%	0.71%	0.16%	370	1.50%	45	130	67	43	280
NBS278	480	480	3.60%	7.5%	33.0%	3.3%	0.68%	0.16%	400	1.40%	51	110	55	42	270
NBS278	530	520	3.50%	7.6%	34.0%	3.5%	0.72%	0.17%	410	1.50%	49	120	56	< 35	260
NBS278	550	550	3.70%	7.5%	36.0%	3.7%	0.75%	0.16%	370	1.60%	61	130	78	< 82	270
NBS278	510	480	3.30%	7.4%	35.0%	3.5%	0.71%	0.16%	380	1.50%	52	110	61	32	230
NBS278	490	510	3.50%	7.4%	36.0%	3.5%	0.72%	0.17%	410	1.50%	44	110	70	46	280
Average	507	506	3.54%	7.46%	34.43%	3.47%	0.71%	0.16%	389	1.49%	49	119	65	41	261
stdev	5.7%	5.3%	3.6%	1.1%	3.7%	4.0%	4.1%	3.0%	4.6%	4.6%	13.5%	7.6%	12.5%	13.0%	7.5%
Certified	500	500	3.59%	7.49%	34.11%	3.45%	0.70%	0.15%	403	1.43%	55	127	64	39	290

Table 6: Results using oxide calculation, where the total matrix is complemented with oxygen through the oxide from of the element.

8 THIN SAMPLE ANALYSIS

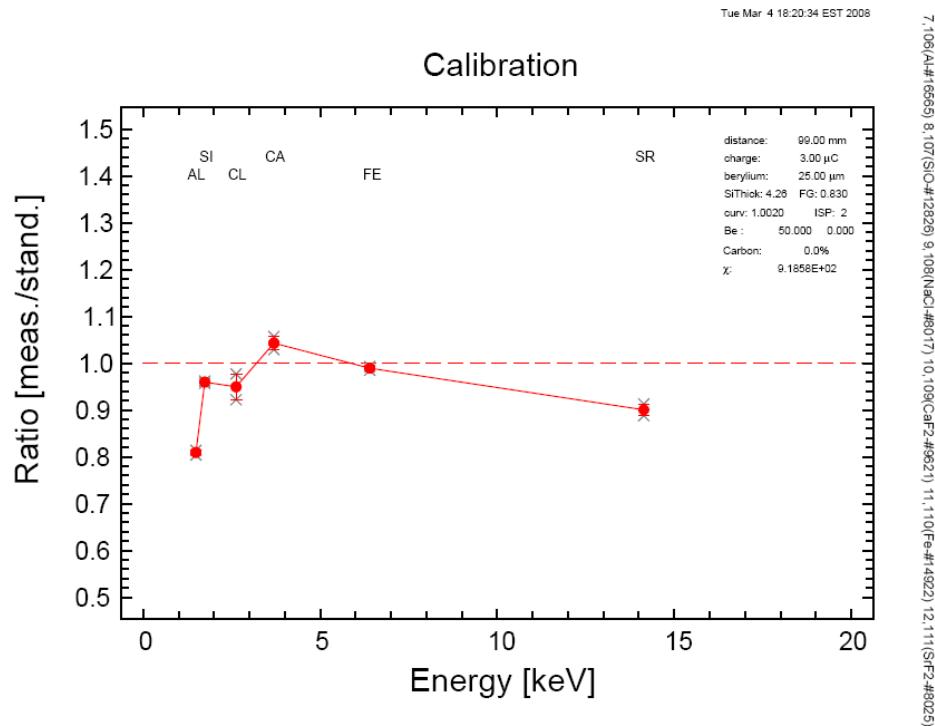


Figure 23: **PIXE** calibration plot. The plot shows that for light elements, the results are generally too low.

technique requiring a reference material. The only way to verify this calibration is to compare it with previous calibration results on the same experimental setup.

After the calibration a number of spectra of the NBS278 standard material are analysed using the iterative and oxide method. The results of both methods are shown in Tab. 5 and Tab. 6. For Al the 1.014 MeV **PIGE** results were selected, since the Al results from **PIXE** are not very reliable, because of the thick filter used in front of the X-ray detector.

Table 5 shows results obtained using the iterative calculation techniques, while the results of table 6 are calculated using the oxide method. Comparison between the 2 tables shows that both approaches give results very close to the certified values.

In a way this is not surprising, because the a standard was used to fine tune the parameters. However, it demonstrate that the automatic calculation of the matrix, works reliably.

8 Thin Sample Analysis

Thin sample analysis is mainly used for thin surfaces on polymers or even graphite. One of its most common use is the analysis of aerosol filters. In fact this is one of the strength of **PIXE**. Because of the short range of the ion beam, for thin layers such as

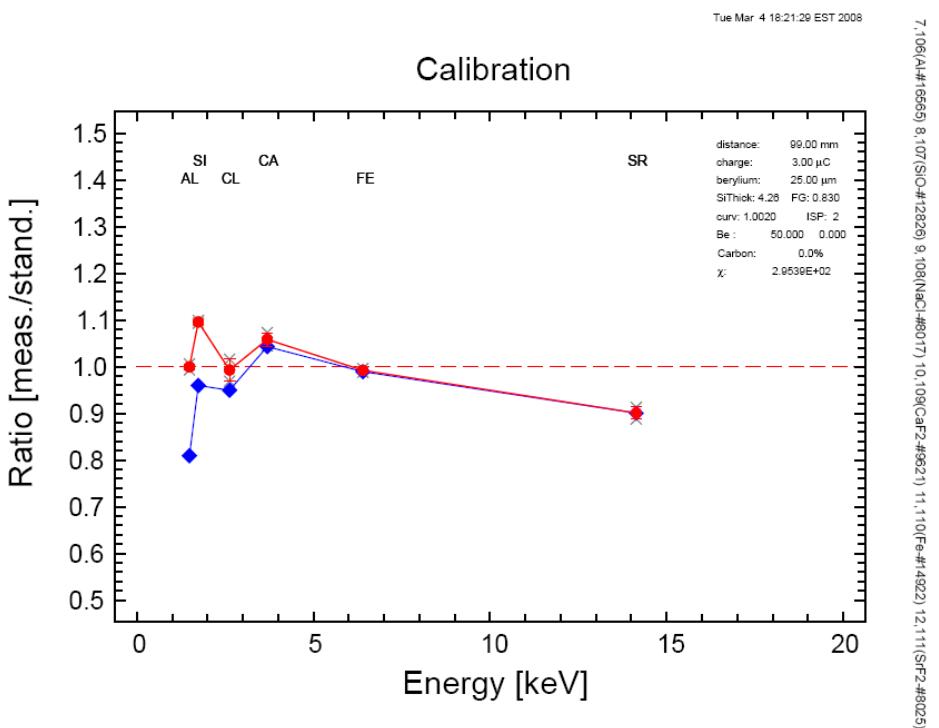


Figure 24: **PIXE** calibration plot, showing the results for various parameter sets..

fine particles filters the yield is still very high and thus very good sensitivity can be achieved.

The analysis of thin samples is easier, since matrix effects as well as the stopping of the beam do not have to be taken into account. However, because the thickness of the sample is unknown, only an area density can be calculated, but no volume concentrations.

Since the so called **PIXE** calibration is only a fine tuning of the analysis parameters, either thin or thick samples can be used for this. **PIGE** on the other hand is a calibration technique and therefore thin samples are required for calibration, if thin samples are analysed. It has to be pointed out that depending on the ion beam energy, the **PIGE** cross sections changes quite significantly. As a consequence of this **PIGE** results are only reliable if the standards used in the calibration and the sample have the same thickness, since no integration over the beam path is performed. This is less important for **PIXE** which does not have strong resonance peaks like **PIGE**.

Thin sample analysis generally can be done with a simple Be filter, thick enough to stop scattered protons from entering the detector. This makes the calibration far easier and more reliable. Fig. 23 shows the calibration using micro-matter reference samples and the nominal parameters for the Be filter thickness. The graph shows that for Si and Al the measured values are lower then the reference values.

To correct this a thin layer of ice was added to the detector parameters. This

8 THIN SAMPLE ANALYSIS

SAMPLE	AL	SI	P	S	CL	K	CA	TI	V	CR	MN	FE	CO	NI	CU	ZN	BR	PBL
ASP0103-10-07Y	0.018*	0.06	0.033	1.045	10.361	2.206	0.211	0	0.002*	0	0.001*	0.045	0.004	0.002	0.001*	0.002*	0.005*	0.009*
ASP0107-10-07R	0.009*	0.125	0.029	2.036	2.961	0.265	0.133	0.012	0.011	0	0.015	0.346	0.003*	0.004	0.008	0.065	0.025	0.027*
ASP0110-10-07Y	0.041	0.172	0.053	3.432	0.048	0.157	0.113	0.006	0.004	0.003	0.006	0.193	0	0.005	0.01	0.019	0.031	0.013*
ASP0114-10-07R	0.078	0.4	0.008*	3.32	4.198	0.415	0.24	0.007	0.008	0.002*	0.014	0.239	0	0.012	0.012	0.044	0.024	0.03
ASP0117-10-07Y	0.214	0.925	0.089	9.427	2.28	0.729	0.465	0.037	0.006	0.008	0.024	0.758	0	0.004*	0.02	0.119	0.04	0.098
ASP0121-10-07R	0.012*	0.244	0.032	2.919	6.189	0.398	0.243	0.01	0.012	0	0.001*	0.2	0.007	0.005	0.008	0.041	0.028	0.04
ASP0124-10-07Y	0.111	0.61	0.141	11.703	0.115	0.461	0.374	0.029	0.007	0.014	0.021	0.426	0.007*	0.012	0.019	0.065	0.042	0.037
ASP0128-10-07R	1.54	2.862	0.021	3.422	11.022	1.488	0.533	0.088	0.005*	0.001*	0.042	1.147	0.009*	0.007	0.02	0.248	0.038	0.092
ASP0803-10-07Y	0.015*	0.112	1.421	1.209	13.622	0.321	0.493	0.011	0.008	0	0.026	0.278	0	0.007	1.235	0.794	0.001*	0.091
ASP0807-10-07R	0.091	0.282	0.057	3.283	5.571	0.487	0.574	0.016	0.005	1.946	0.005*	0.002*	0.027	0.027	0.21	0.058	0.032	0.041
ASP0810-10-07Y	0.324	1.069	0.003*	2.258	1.341	0.209	0.671	0.055	0.013	0.017	0.04	1.119	0.017	0.007	0.023	0.055	0.011*	0.041
ASP0814-10-07R	0.166	0.792	0.02	6.347	4.007	0.894	1.095	0.03	0.039	0.005	0.124	3.913	0.012*	0.01	0.03	0.993	0.07	0.123
ASP0817-10-07Y	0.498	1.866	0.149	15.244	3.547	1.477	2.236	0.065	0.047	0.005*	0.16	5.9	0.010*	0.02	0.081	0.484	0.053	0.24
ASP0821-10-07R	0.025*	0.269	0.039	5.032	9.33	0.853	0.851	0.011	0.019	0.015	0.073	2.331	0	0.005*	0.001*	0.5	0.043	0.113
ASP0824-10-07Y	0.202	0.821	0.628	15.743	0.906	1.314	1.308	0.046	0.04	0.027	0.113	3.574	0.024	0.018	0.215	1.035	0.101	0.312
ASP0828-10-07R	0.361	1.463	0.02	3.96	10.668	1.272	0.927	0.045	0.006*	0	0.078	1.953	0.011*	0.003*	0.009	0.403	0.045	0.052
ASP1007-10-07R	0.091	0.249	0.057	1.814	15.701	0.35	0.416	0.004*	0.018	0	0.007	0.442	0	0.009	0.015	0.033	0.047	0.023*
ASP1010-10-07Y	0.078	0.254	0.006*	1.403	5.791	0.374	0.209	0.011	0.008	0.006	0.621	0.269	0.012	0.014	0.009	0.081	0.025	0.043
ASP1014-10-07R	1.041	1.014	0.022	3.181	0.384	0.379	0.319	0.037	0.027	0.014	0.333	1.378	0.001*	0.007	0.04	0.291	0.019	0.114
ASP1021-10-07R	0.72	1.204	0.073	7.701	1.634	0.881	0.362	0.045	0.026	0.022	1.05	0.649	0	0.005	0.065	0.233	0.062	0.044
ASP1024-10-07Y	0.809	2.391	0.098	7.607	7.537	1.048	0.876	0.121	0.016	0.053	8.911	2.932	0	0.015	0.071	0.815	0.036	0.123
ASP1028-10-07R	0.105	0.365	0.023	3.914	7.741	0.557	0.34	0.008	0.025	0.012	0.459	2.297	0.004*	0.009	0.003*	0.221	0.02	0.051
ASP1103-10-07Y	4.52	13.255	0	14.454	10.003	3.146	3.494	0.375	0.043	0.018	2.401	6.691	0.002*	0.017	0.079	0.919	0.12	4.026
ASP1107-10-07R	0.711	1.949	0.001*	2.614	11.677	0.98	0.592	0.049	0.005*	0	0.195	0.505	0	0.003*	0.008	0.306	0.052	0.032
ASP1110-10-07Y	0.05	0.078	0.016	1.362	10.004	0.574	0.222	0.006	0	0	0.002*	0.054	0.004	0.009	0.004	0.016	0.018	0.024
ASP1114-10-07R	0.138	0.253	0.056	3.571	3.099	1.424	0.089	0.015	0.011	0.003*	0.067	0.07	0	0.005	0.007	0.052	0.05	0.157
ASP1117-10-07Y	2.669	0.32	0.016	3.232	2.852	0.894	0.188	0.014	0.004	0.007	0.476	0.182	0.003*	0.007	0.008	0.061	0.022	0.139
ASP1121-10-07R	4.04	0.334	0.06	3.462	6.887	0.991	0.286	0.011	0.024	0.005	0.61	1.131	0.002*	0.01	0.006	0.02	0.023	0.165
ASP1124-10-07Y	0.476	0.375	0.038	5.669	15.942	1.295	0.606	0.013	0.002*	0	0.419	0.151	0.002*	0.002*	0.005	0.026	0.049	0.213
ASP1128-10-07R	0.16	0.076	0.087	2.092	11.625	1.083	0.288	0.007	0.001*	0.001*	0.026	0.016	0.003	0.003	0.002*	0.034	0.061	0.04
ASP1803-10-07Y	0.005*	0.167	0.024	1.465	9.346	0.576	0.244	0.002*	0.001*	0	0.017	1.08	0.006	0.006	0.009	0.038	0.021	0.004*
ASP1807-10-07R	0.030*	0.048	0.043	2.131	24.415	0.485	0.007	0.014	0	0.013	0.012	0.005	0.003	0.007	0.004	0.009	0.005*	0.005
ASP1817-10-07Y	0	0.1	1.05	2.117	5.293	0.426	0.246	0.011	0	0.02	0.009	0.227	0	0.002*	0.087	0.096	0	0.052
ASP1821-10-07R	0.024	0.148	0.010*	1.528	1.269	0.397	0.111	0.007	0	0.003	0.011	0.168	0.007	0.411	0.007*	0.059	0.027	0.067
ASP1824-10-07Y	0.131	0.389	0.05	2.04	0.031	0.346	0.12	0.014	0.006	0.013	0.01	0.245	0.002*	0.009	0.007	0.031	0.026	0.062
ASP1828-10-07R	0.194	0.716	0.025	3.462	2.933	0.747	0.251	0.033	0.013	0.004	0.016	0.329	0.005*	0.013	0.014	0.07	0.048	0.069
ASP2303-10-07Y	0.351	1.333	0.09	5.926	0.022	0.225	0.045	0.001*	0.001*	0.006	0.43	0	0	0.013	0.056	0.022	0.05	0.022
ASP2307-10-07R	0.101	0.511	0.031	2.54	5.461	0.77	0.227	0.021	0.001*	0.003*	0.003*	0.317	0.007	0.008	0.013	0.084	0.036	0.044
ASP2310-10-07Y	0.291	1.115	0.205	13.97	0.08	0.62	0.401	0.047	0	0.005	0.014	0.477	0.008	0.007	0.014	0.079	0.03	0.043
ASP2314-10-07R	0.269	1.015	0.008*	2.882	9.807	1.075	0.366	0.03	0.008	0.003*	0.01	0.27	0	0	0.01	0.027	0.024	0.001*

Table 7: Results for thin samples in ng/cm².

RUN=091 pixe Aerosols sep07 22/10/07 5:44:13 PM

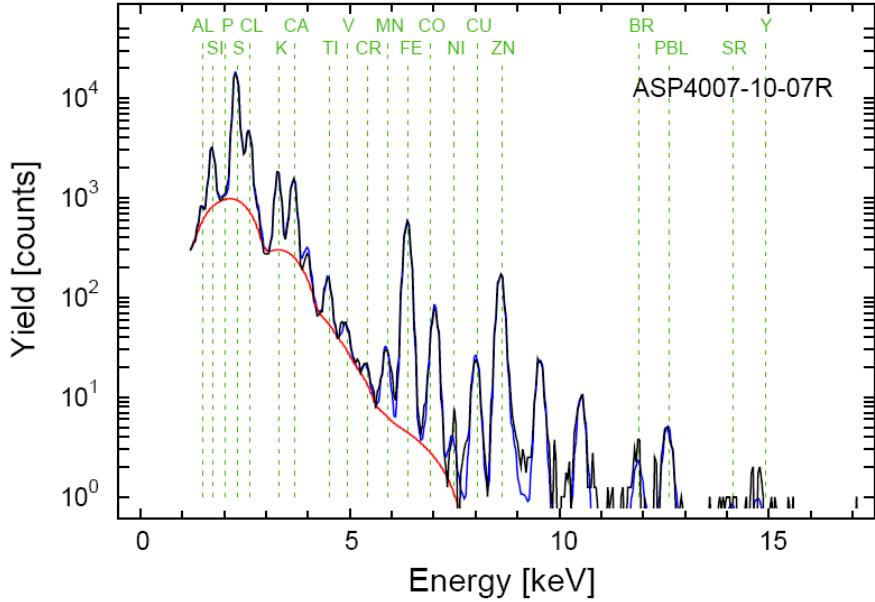


Figure 25: `batty` fit of an aerosol filter sample.

changes only the concentration of the light elements and the results of a rerun of the calibration is shown in Fig. 24. This shows very good agreement between the measured and the reference values. For all the elements the spread is about 10% which is quite wide. However, it is well known that in the micro-matter samples the reference value for Sr is overestimated.

Figure 25 shows a fit for a typical spectrum from an aerosol filter samples. The spectrum shows a large number of peaks, all of which are quite well fitted.

Table 7 shows the results of for some thin samples. The results are given in ng/cm². The table shows that a large number of elements can be analysed simultaneously with high sensitivity. Values marked with a star indicate that the result is below the minimum detection limit (MDL).

8 THIN SAMPLE ANALYSIS

Appendix

This section is added for completeness and debugging purposes. It contains and describes the run control files for the **PIXAN** package programs **batty**, **thin** and **thick** as well for **ptanal**. All the above programs are written in such a way that they can analyse a number of spectra contained in single file in one session using the same parameters. Individual spectra are identified by their block number, which is the first number in the second line of the spectrum.

This approach was not used in the **doiba** package, since it uses the same parameters for all spectra. To overcome this limitation, each spectrum is run individually through the programs of the **PIXAN** package.

The information in this section is not required to run the **doiba** package. However, it may be used to debug any problems in the analysis program.

A PIXAN package

The **doiba** package at the moment does both **PIXE** and **PIGE** analysis, whereby both are combined to produce a result based on both. The **PIXE** analysis part is based on the **PIXAN** package, which performs the main calculations. The **PIXAN** package is comprised of two main parts **batty** and **conc**. **Batty** itself does the fitting of the spectra and provides peak areas for the X-ray peaks. These areas are used by **concs** to calculate the concentrations.

A.1 BATTY

batty is executed from the command line without any command line parameters. The run control file is entered after the prompt. The listing below shows how **batty** is run, the run control file in this case has the syntax used by **doiba**.

Example of command line execution of **batty**

```
boson:~/ANALYSIS/test$ batty98
Please enter your plotting choice
screen is type 1
zeta      2
laser     3

3

Enter the control file for running
The default is runbatty.run  If you wish that use CR
If you want the demonstration enter demorun.run

28feb08.brc
```

A PIXAN PACKAGE

BATTY Configuration File

The batty run control file has a fixed format. An example is show below

Example of **batty** run control file

```

16      1     -1      7
pixe031.plot
0.019900   -0.050000
0.050000   0.003000   0.003000   1.000000
25.000000   0.300000   0.020000   4.260000   0.83000   0.000000
9
2
1    0.048   0.000000
2    1.86    0.034
5
1.002      3
1      1
pixe031.area
NOSE
SUME
5
1.0000   20.0000
6    1
FE AL SI P S CL K CA TI V CR MN NI CU ZN
GA GE AS RB SR Y ZR NB PBL END
1
/home/usr/analysis/pixe/pixe031.rpt
1113
-1

```

Line 1: The first line contains four integer numbers, *MODE*, *IPLOT*, *IDELY*, *IBAKC*. *MODE* describes the plotting mode, *IPLOT* is > 1 if plot data should be written and the filename for the plot has to follow in the next line. If the plot is to be displayed on the screen *IDELY* is the time the plot will be displayed on the screen. *IBACKC* is the background colour for the plot.

Line 1a: When *IPLOT* is greater zero the the next line provides the name for the file to which the plot data will be written.

Line 2: The next line in the file contains *DELETE* and *CALNT* the energy calibration for the spectra.

$$e = \text{DELETE} * i + \text{CALNT} \quad (2)$$

Line 3: This line contains *XBE*, *XSI*, *XAU*, *XTHICK*, *FG*, *XICE*.

Line 4:

This line contains *IFILT*, which determines the filter

<i>IFILT</i>	Filter Type
0	no filter
1	Mylar filter
2	Perspex
3	Kapton
4	Beryllium
5	Graphite
6	Aluminium
7	Helium
8	Air
9	define layers from the above list
10	define your own including layers

Line 4a: When *IFILT* is greater than 1 and below 9 the next line contains *THICK* and *HOLE*, the thickness of the filter and the hole size in the filter.

When *IFILT* is 9 the next line gives *NLAYER* the number of layers in the filter. This will be followed by *NLAYER* lines of the format *THICK HOLE*.

Line 5: Line 6 gives *IBAK* the background. *IBAK* can have values from 1 to 5, which have the following meaning.

<i>IBAK</i>	
1	a background spectrum drawn from the same dataset as the experimental data is used
2	values for the polynomial fit are read in
3	polynomial parameters are calculated
4	polynomial parameters are read in with the spectrum
5	the peak filing background is used

Line 5a-1: With *IBAK* 1

Line 5a-2: With *IBAK* 2 the next line contains *ENORT* and *NORD* which is followed by:

Line 5b-2: With *IBAK* 2 this is followed by *POLY(I), I=1,NORD+1*

A PIXAN PACKAGE

Line 5a-3: With *IBAK* 3 or 4 the next line contains *ENORT* and *NORD*.

Line 5a-5: With *IBAK* 5 the next line contains *CURV* and *ISP*, where *CURV* is the curvature parameter and *ISP* is the low energy spacing for the peak filing background.

Line 6: The next line contains *IREP* and *IFILE*, where *IREP* determines how the program handles negative peak areas. If *IREP* is positive negative areas are deleted from the fit and the calculation is repeated. *IFILE* determines whether the calculated peak areas are output onto disk, so that they can be used for further calculations. If *IFILE* is positive, then element names and peak areas are placed on disk and the next line following contains the filename

Line 6a: If *IFILE* is greater than 0 then this line contains the filename to which the peak areas are written.

Line 7: *TESTSELF* self absorption This is used to set whether self absorption effects are included in the background calculation and relative intensities. If this is set to SELF, self absorption effect corrections are made. If it is set to ASI these corrections are not made and the spectrum is not divided by the detector efficiency before the minima are found for determining the background polynomial. If Selftest is set to neither of these values, no self absorption corrections are made.

Line 7a: *NMAT* If *TESTSELF*=SELF it is followed by *NMAT* the number of major components.

Line 7b: *TSEL*, *CONC* The name for each major component and its concentration. (6 elements to a line).

Line 8: *SUME* The next line contains *SUME* which can have the values *SUME* and *NOSU*. If *SUME* equals *SUME* then an element called *SUME* is included in the fit and the next line contains the number *NSUMIN*, which is the number of elements that will be summed over.

Line 8a: *NSUMIN* *NSUMIN* is the number of elements included in the calculation of sumpeaks.

Line 9: *IFIX*, *ITAIL*

Line 10: *ELO*, *EHI* Lower and upper limit of the **batty** fit.

A.2 CONCS

Line 11: Element list The next line is the list of elements. This list can be broken over more than one line and has to be terminated by END after the last element. All elements have to be listed in capital letters. To include L and M lines in the list the element name is appended by an L or M.

Line 12: A value below 2 indicates that the next line contains the spectrum file name.

Line 12b: Spectrum File Name Spectrum File Name with full path.

Line 13: Block Numbers A list of block numbers of the spectra to be analysed by [batty](#). The list is terminated by -1.

A.2 CONCS

CONCS Configuration File

Example of [concs](#) run control file

```
-1      1
pixe031.area
 93.000    0.00000   45.00000    4.00000
 2.5     0.5     15
 25.000000   0.300000   0.020000   4.260000   0.83000   0.000000
 9
 2
 1     0.048   0.000000
 2     1.86    0.034
AL SI P S CL K CA TI V CR MN FE NI CU ZN
GA GE AS RB SR Y ZR NB PBL END
Put any comment here
C 0 END
0.5 0.5
```

Line 1: *IPRT*, *IOUT* This line contains *IPRT* and *IOUT*. *IPRT* controls the output of [concs](#). If *IPRT* is negative only the thick target yield is printed. If *IPRT* is positive a comprehensive output is produced. *IOUT* controls the input of [concs](#). If *IOUT* is greater than zero, the next line contains file and path for the area input file, which is the [batty](#) output file.

Line 1a: Area data filename This line contains the path and name of the area input file, if *IOUT* is greater than zero.

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Line 2: *DIST, THTIN, THEOUT, DIAM* The next line *DIST, THTIN, THEOUT, DIAM*.

Line 3: *EHI, ELO, CHAR* *EHI* and *ELO* and the upper and lower limit of the beam energy over which the X-ray yield is integrated. *CHAR* is the total charge of analysis.

Line 4: *XBE, XSI, XAU, XTHICK, FG, XICE* The next line is *XBE, XSI, XAU, XTHICK, FG, XICE*.

Line 5:

This and subsequent lines defines the filter *IFILT*. The same format as in batty is used.

Line 6: Element list The next line is the list of elements. This list can be broken over more than one line and has to be terminated by END. All elements have to be listed in capital letters.

Line 7: Matrix Composition Elements This line contains the list of the matrix elements and is terminated by END. The elements have to be entered in capital letters.

Line 7b: The next line contains the relative concentration of the matrix elements, in the same order as the elements in the above line. This line does not have to be terminated by END.

In [concs](#) a separate file is needed that selects the blocknumbers, to be analysed.

A.3 PIXAN data files

The PIXAN package uses 4 data input files dset2, dset3, dset4 and dset5. dset2 contains a list characteristic X-ray energies and intensities for all elements. The format is Element and number of characteristic X-ray line entries in file, followed by lines with the X-ray energy and the relative line intensity. In most cases the intensity for K_{α} of L_{α} is set to 1.0. The list has separate entries for K, L and M lines.

Format of dset2 data file

NA	1
1.041	1.000
MG	1
1.253	1.000
AL	1
1.486	1.000
SI	2
1.736	1.000
1.839	0.027
P	2
2.013	1.000
2.139	0.043
S	2
2.307	1.000
2.464	0.059
CL	2
2.621	1.000
2.816	0.082
AR	2
2.955	1.000
3.190	0.105

A.3 PIXAN data files

K	2		
3.312	1.000	3.589	0.117
CA	2		
3.690	1.000	4.012	0.128

A listing of the data file dset3 is shown below.

Listing of dset3 data file

H	1.000		
0.5977000D+03	0.1440000D+01	0.2426000D+03	0.1200000D+05
0.1159000D+00	0.5099000D-03	0.5436000D+05	-0.5052000D+01
0.2049000D+01	-0.3044000D+00	0.1966000D-01	-0.4659000D-03
0.0	0.0	0.1360000D-01	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
HE	2.000		
0.1505000D+03	0.1397000D+01	0.4845000D+03	0.5873000D+04
0.5225000D-01	0.1020000D-02	0.2451000D+05	-0.2158000D+01
0.8278000D+00	-0.1172000D+00	0.7259000D-02	-0.1660000D-03
0.0	0.0	0.2500000D-01	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
LI	3.000		
0.8683000D+02	0.1600000D+01	0.7256000D+03	0.3013000D+04
0.4578000D-01	0.1530000D-02	0.2147000D+05	-0.5831000D+00
0.5620000D+00	-0.1183000D+00	0.9298000D-02	-0.2498000D-03
0.0	0.0	0.5500000D-01	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
BE	4.000		
0.6685000D+02	0.2590000D+01	0.9660000D+03	0.1538000D+03
0.3475000D-01	0.2039000D-02	0.1630000D+05	0.2779000D+00
0.1745000D+00	-0.5684000D-01	0.5155000D-02	-0.1488000D-03
0.0	0.0	0.1120000D+00	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
B	5.000		
0.5573000D+02	0.2815000D+01	0.1206000D+04	0.1060000D+04
0.2855000D-01	0.2549000D-02	0.1345000D+05	-0.2445000D+01
0.1283000D+01	-0.2205000D+00	0.1560000D-01	-0.3930000D-03
0.0	0.0	0.1880000D+00	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
C	6.000		
0.5016000D+02	0.2989000D+01	0.1445000D+04	0.9572000D+03
0.2819000D-01	0.3059000D-02	0.1322000D+05	-0.4380000D+01
0.2044000D+01	-0.3283000D+00	0.2221000D-01	-0.5417000D-03
0.0	0.0	0.2840000D+00	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
N	7.000		
0.4302000D+02	0.3350000D+01	0.1683000D+04	0.1900000D+04
0.2513000D-01	0.3569000D-02	0.1179000D+05	-0.5054000D+01
0.2325000D+01	-0.3713000D+00	0.2506000D-01	-0.6109000D-03
0.0	0.0	0.4010000D+00	0.2000000D+03
0.0	0.0	0.2920000D+01	0.0
0.0	0.3070000D+01	0.0	0.0
0.5400000D-02			
O	8.000		

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	0.3766000D+02	0.3000000D+01	0.1920000D+04	0.2000000D+04
	0.2230000D-01	0.4079000D-02	0.1046000D+05	-0.6734000D+01
	0.3019000D+01	-0.4748000D+00	0.3171000D-01	-0.7669000D-03
	0.0	0.0	0.5320000D+00	0.2000000D+03
	0.0	0.0	0.2920000D+01	0.0
	0.0	0.3070000D+01	0.0	0.0
	0.5400000D-02			
F	9.000			
	0.3171000D+02	0.2352000D+01	0.2157000D+04	0.2634000D+04
	0.1816000D-01	0.4589000D-02	0.8517000D+04	-0.5571000D+01
	0.2449000D+01	-0.3781000D+00	0.2483000D-01	-0.5919000D-03
	0.0	0.0	0.6870000D+00	0.2000000D+03
	0.0	0.0	0.2920000D+01	0.0
	0.0	0.3070000D+01	0.0	0.0
	0.5400000D-02			
NE	10.000			
	0.2985000D+02	0.2199000D+01	0.2393000D+04	0.2699000D+04
	0.1568000D-01	0.5099000D-02	0.7353000D+04	-0.4408000D+01
	0.1879000D+01	-0.2814000D+00	0.1796000D-01	-0.4168000D-03
	0.0	0.0	0.8670000D+00	0.2000000D+03
	0.0	0.0	0.2920000D+01	0.0
	0.0	0.3070000D+01	0.0	0.0
	0.5400000D-02			
NA	11.000			
	0.2621000D+02	0.2869000D+01	0.2628000D+04	0.1854000D+04
	0.1472000D-01	0.5609000D-02	0.6905000D+04	-0.4959000D+01
	0.2073000D+01	-0.3054000D+00	0.1921000D-01	-0.4403000D-03
	0.0	0.6300000D-01	0.1072000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
MG	12.000			
	0.2478000D+02	0.4293000D+01	0.2862000D+04	0.1009000D+04
	0.1397000D-01	0.6118000D-02	0.6551000D+04	-0.5510000D+01
	0.2266000D+01	-0.3295000D+00	0.2047000D-01	-0.4637000D-03
	0.0	0.8910000D-01	0.3050000D+00	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
AL	13.000			
	0.2233000D+02	0.4739000D+01	0.2766000D+04	0.1645000D+03
	0.2023000D-01	0.6628000D-02	0.6309000D+04	-0.6061000D+01
	0.2460000D+01	-0.3535000D+00	0.2173000D-01	-0.4871000D-03
	0.0	0.1180000D+00	0.1559000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
SI	14.000			
	0.2145000D+02	0.4700000D+01	0.3329000D+04	0.5500000D+03
	0.1321000D-01	0.7138000D-02	0.6194000D+04	-0.6294000D+01
	0.2538000D+01	-0.3628000D+00	0.2220000D-01	-0.4956000D-03
	0.0	0.1491000D+00	0.1838000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
P	15.000			
	0.1945000D+02	0.3647000D+01	0.3561000D+04	0.1560000D+04
	0.1267000D-01	0.7648000D-02	0.5942000D+04	-0.6527000D+01
	0.2616000D+01	-0.3721000D+00	0.2267000D-01	-0.5040000D-03
	0.0	0.1890000D+00	0.2142000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
S	16.000			
	0.1879000D+02	0.3891000D+01	0.3792000D+04	0.1219000D+04
	0.1211000D-01	0.8158000D-02	0.5678000D+04	-0.6761000D+01

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	0.2694000D+01	-0.3814000D+00	0.2314000D-01	-0.5125000D-03
	0.0	0.2290000D+00	0.2472000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
CL	17.000			
	0.1699000D+02	0.5714000D+01	0.4023000D+04	0.8786000D+03
	0.1178000D-01	0.8668000D-02	0.5524000D+04	-0.6994000D+01
	0.2773000D+01	-0.3907000D+00	0.2361000D-01	-0.5209000D-03
	0.0	0.2700000D+00	0.2822000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
AR	18.000			
	0.1508000D+02	0.6500000D+01	0.4253000D+04	0.5300000D+03
	0.1123000D-01	0.9178000D-02	0.5268000D+04	-0.7227000D+01
	0.2851000D+01	-0.4000000D+00	0.2407000D-01	-0.5294000D-03
	0.0	0.3130000D+00	0.3202000D+01	0.2000000D+03
	0.0	0.2740000D+01	0.2790000D+01	0.0
	0.3030000D+01	0.2730000D+01	0.0	0.5330000D-03
	0.1380000D-01			
K	19.000			
	0.1541000D+02	0.5833000D+01	0.4482000D+04	0.5457000D+03
	0.1129000D-01	0.9687000D-02	0.5295000D+04	-0.7440000D+01
	0.2923000D+01	-0.4094000D+00	0.2462000D-01	-0.5411000D-03
	0.0	0.2940000D+00	0.3607000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
CA	20.000			
	0.1503000D+02	0.6252000D+01	0.4710000D+04	0.5533000D+03
	0.1112000D-01	0.1020000D-01	0.5214000D+04	-0.7653000D+01
	0.2995000D+01	-0.4187000D+00	0.2516000D-01	-0.5529000D-03
	0.2500000D-01	0.3460000D+00	0.4038000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
SC	21.000			
	0.1340000D+02	0.5884000D+01	0.4938000D+04	0.5609000D+03
	0.9995000D-02	0.1071000D-01	0.4688000D+04	-0.8012000D+01
	0.3123000D+01	-0.4350000D+00	0.2605000D-01	-0.5707000D-03
	0.7000000D-02	0.4020000D+00	0.4496000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
TI	22.000			
	0.1258000D+02	0.5496000D+01	0.5165000D+04	0.5685000D+03
	0.9474000D-02	0.1122000D-01	0.4443000D+04	-0.8371000D+01
	0.3251000D+01	-0.4513000D+00	0.2694000D-01	-0.5886000D-03
	0.4000000D-02	0.4560000D+00	0.4965000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
V	23.000			
	0.1183000D+02	0.5055000D+01	0.5391000D+04	0.9523000D+03
	0.9117000D-02	0.1173000D-01	0.4276000D+04	-0.8731000D+01
	0.3379000D+01	-0.4676000D+00	0.2783000D-01	-0.6064000D-03
	0.2000000D-02	0.5130000D+00	0.5465000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
CR	24.000			
	0.1159000D+02	0.4489000D+01	0.5616000D+04	0.1336000D+04
	0.8413000D-02	0.1224000D-01	0.3946000D+04	-0.9090000D+01
	0.3507000D+01	-0.4838000D+00	0.2872000D-01	-0.6243000D-03
	0.2000000D-02	0.5740000D+00	0.5989000D+01	0.2000000D+03

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	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
MN	25.000			
	0.1097000D+02	0.3907000D+01	0.5725000D+04	0.1461000D+04
	0.8829000D-02	0.1275000D-01	0.3785000D+04	-0.9449000D+01
	0.3635000D+01	-0.5001000D+00	0.2961000D-01	-0.6421000D-03
	0.3000000D-02	0.6400000D+00	0.6540000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
FE	26.000			
	0.1079000D+02	0.3963000D+01	0.6065000D+04	0.1243000D+04
	0.7782000D-02	0.1326000D-01	0.3650000D+04	-0.9809000D+01
	0.3763000D+01	-0.5164000D+00	0.3050000D-01	-0.6600000D-03
	0.4000000D-02	0.7080000D+00	0.7112000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
CO	27.000			
	0.1022000D+02	0.3535000D+01	0.6288000D+04	0.1372000D+04
	0.7361000D-02	0.1377000D-01	0.3453000D+04	-0.1017000D+02
	0.3891000D+01	-0.5327000D+00	0.3139000D-01	-0.6779000D-03
	0.3000000D-02	0.7790000D+00	0.7709000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
NI	28.000			
	0.1026000D+02	0.4004000D+01	0.6205000D+04	0.5551000D+03
	0.8763000D-02	0.1428000D-01	0.3297000D+04	-0.1053000D+02
	0.4019000D+01	-0.5490000D+00	0.3229000D-01	-0.6957000D-03
	0.4000000D-02	0.8550000D+00	0.8333000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
CU	29.000			
	0.9482000D+01	0.4175000D+01	0.4673000D+04	0.3878000D+03
	0.2188000D-01	0.1479000D-01	0.3174000D+04	-0.1118000D+02
	0.4252000D+01	-0.5791000D+00	0.3399000D-01	-0.7314000D-03
	0.2000000D-02	0.9320000D+00	0.8979000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
ZN	30.000			
	0.9217000D+01	0.4750000D+01	0.6953000D+04	0.2952000D+03
	0.6809000D-02	0.1530000D-01	0.3194000D+04	-0.1157000D+02
	0.4394000D+01	-0.5980000D+00	0.3506000D-01	-0.7537000D-03
	0.8000000D-02	0.1021000D+01	0.9659000D+01	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
GA	31.000			
	0.8642000D+01	0.5697000D+01	0.7173000D+04	0.2026000D+03
	0.6725000D-02	0.1581000D-01	0.3154000D+04	-0.1195000D+02
	0.4537000D+01	-0.6169000D+00	0.3613000D-01	-0.7759000D-03
	0.1000000D-01	0.1117000D+01	0.1036800D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
GE	32.000			
	0.8300000D+01	0.6300000D+01	0.6496000D+04	0.1100000D+03
	0.9689000D-02	0.1632000D-01	0.3097000D+04	-0.1234000D+02
	0.4680000D+01	-0.6358000D+00	0.3721000D-01	-0.7981000D-03
	0.1000000D-01	0.1218000D+01	0.1110400D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03

A.3 PIXAN data files

	0.3120000D-01			
AS	33.000			
	0.8042000D+01	0.6012000D+01	0.7611000D+04	0.2925000D+03
	0.6447000D-02	0.1683000D-01	0.3024000D+04	-0.1272000D+02
	0.4823000D+01	-0.6547000D+00	0.3828000D-01	-0.8203000D-03
	0.1000000D-01	0.1325000D+01	0.1186800D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
SE	34.000			
	0.7630000D+01	0.6656000D+01	0.7395000D+04	0.1175000D+03
	0.7684000D-02	0.1734000D-01	0.3006000D+04	-0.1311000D+02
	0.4965000D+01	-0.6735000D+00	0.3935000D-01	-0.8425000D-03
	0.5700000D-01	0.1436000D+01	0.1265800D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
BR	35.000			
	0.7540000D+01	0.6335000D+01	0.8046000D+04	0.3652000D+03
	0.6244000D-02	0.1785000D-01	0.2928000D+04	-0.1340000D+02
	0.5083000D+01	-0.6906000D+00	0.4042000D-01	-0.8675000D-03
	0.1000000D+00	0.1550000D+01	0.1347400D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
KR	36.000			
	0.7190000D+01	0.7250000D+01	0.8262000D+04	0.2200000D+03
	0.6087000D-02	0.1836000D-01	0.2855000D+04	-0.1369000D+02
	0.5200000D+01	-0.7076000D+00	0.4150000D-01	-0.8925000D-03
	0.9400000D-01	0.1675000D+01	0.1432200D+02	0.2000000D+03
	0.2440000D+01	0.2700000D+01	0.2660000D+01	0.3470000D+01
	0.2900000D+01	0.2470000D+01	0.2730000D-04	0.9590000D-03
	0.3120000D-01			
RB	37.000			
	0.7049000D+01	0.6429000D+01	0.8478000D+04	0.2929000D+03
	0.6087000D-02	0.1886000D-01	0.2855000D+04	-0.1392000D+02
	0.5266000D+01	-0.7140000D+00	0.4173000D-01	-0.8943000D-03
	0.1100000D+00	0.1806000D+01	0.1866000D+01	0.1520100D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
SR	38.000			
	0.6876000D+01	0.7159000D+01	0.8693000D+04	0.3303000D+03
	0.6003000D-02	0.1937000D-01	0.2815000D+04	-0.1414000D+02
	0.5331000D+01	-0.7205000D+00	0.4196000D-01	-0.8962000D-03
	0.1330000D+00	0.1940000D+01	0.2007000D+01	0.1610500D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
Y	39.000			
	0.6777000D+01	0.7234000D+01	0.8907000D+04	0.3678000D+03
	0.5889000D-02	0.1988000D-01	0.2762000D+04	-0.1436000D+02
	0.5397000D+01	-0.7269000D+00	0.4219000D-01	-0.8980000D-03
	0.1570000D+00	0.2079000D+01	0.2145000D+01	0.1703700D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
ZR	40.000			
	0.6605000D+01	0.7603000D+01	0.9120000D+04	0.4052000D+03
	0.5765000D-02	0.2039000D-01	0.2704000D+04	-0.1459000D+02
	0.5463000D+01	-0.7333000D+00	0.4242000D-01	-0.8998000D-03
	0.1800000D+00	0.2223000D+01	0.2307000D+01	0.1799800D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
NB	41.000			

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	0.6485000D+01	0.7791000D+01	0.9333000D+04	0.4427000D+03
	0.5587000D-02	0.2090000D-01	0.2621000D+04	-0.1622000D+02
	0.6094000D+01	-0.8225000D+00	0.4791000D-01	-0.1024000D-02
	0.2050000D+00	0.2371000D+01	0.2465000D+01	0.1898600D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
MO	42.000			
	0.6280000D+01	0.7248000D+01	0.9545000D+04	0.4802000D+03
	0.5367000D-02	0.2141000D-01	0.2517000D+04	-0.1785000D+02
	0.6725000D+01	-0.9116000D+00	0.5339000D-01	-0.1148000D-02
	0.2270000D+00	0.2520000D+01	0.2625000D+01	0.2000200D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
TC	43.000			
	0.6086000D+01	0.7671000D+01	0.9756000D+04	0.5176000D+03
	0.5315000D-02	0.2192000D-01	0.2493000D+04	-0.1796000D+02
	0.6752000D+01	-0.9135000D+00	0.5341000D-01	-0.1147000D-02
	0.2530000D+00	0.2677000D+01	0.2795000D+01	0.2105400D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
RU	44.000			
	0.5961000D+01	0.6887000D+01	0.9966000D+04	0.5551000D+03
	0.5151000D-02	0.2243000D-01	0.2416000D+04	-0.1807000D+02
	0.6779000D+01	-0.9154000D+00	0.5342000D-01	-0.1145000D-02
	0.2790000D+00	0.2837000D+01	0.2966000D+01	0.2211800D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
RH	45.000			
	0.5855000D+01	0.6677000D+01	0.1018000D+05	0.5925000D+03
	0.4919000D-02	0.2294000D-01	0.2307000D+04	-0.1818000D+02
	0.6806000D+01	-0.9173000D+00	0.5343000D-01	-0.1143000D-02
	0.3070000D+00	0.3003000D+01	0.3146000D+01	0.2322400D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
PD	46.000			
	0.5663000D+01	0.5900000D+01	0.1038000D+05	0.6300000D+03
	0.4758000D-02	0.2345000D-01	0.2231000D+04	-0.1828000D+02
	0.6833000D+01	-0.9192000D+00	0.5345000D-01	-0.1142000D-02
	0.3350000D+00	0.3173000D+01	0.3330000D+01	0.2435000D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
AG	47.000			
	0.5585000D+01	0.6354000D+01	0.7160000D+04	0.3376000D+03
	0.1394000D-01	0.2396000D-01	0.2193000D+04	-0.1839000D+02
	0.6860000D+01	-0.9211000D+00	0.5346000D-01	-0.1140000D-02
	0.3670000D+00	0.3351000D+01	0.3524000D+01	0.2551400D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
CD	48.000			
	0.5360000D+01	0.6554000D+01	0.1080000D+05	0.3555000D+03
	0.4626000D-02	0.2447000D-01	0.2170000D+04	-0.1862000D+02
	0.6915000D+01	-0.9243000D+00	0.5340000D-01	-0.1134000D-02
	0.4040000D+00	0.3537000D+01	0.3727000D+01	0.2671100D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
IN	49.000			
	0.5247000D+01	0.7024000D+01	0.1101000D+05	0.3709000D+03
	0.4540000D-02	0.2498000D-01	0.2129000D+04	-0.1885000D+02

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	0.6969000D+01	-0.9275000D+00	0.5335000D-01	-0.1127000D-02
	0.4430000D+00	0.3730000D+01	0.3938000D+01	0.2794000D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
SN	50.000			
	0.5076000D+01	0.7227000D+01	0.1121000D+05	0.3864000D+03
	0.4474000D-02	0.2549000D-01	0.2099000D+04	-0.1907000D+02
	0.7024000D+01	-0.9308000D+00	0.5329000D-01	-0.1121000D-02
	0.4850000D+00	0.3929000D+01	0.4156000D+01	0.2920000D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
SB	51.000			
	0.4949000D+01	0.8480000D+01	0.8608000D+04	0.3480000D+03
	0.9074000D-02	0.2600000D-01	0.2069000D+04	-0.1957000D+02
	0.7225000D+01	-0.9603000D+00	0.5518000D-01	-0.1165000D-02
	0.5000000D+00	0.4132000D+01	0.4381000D+01	0.3049100D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
TE	52.000			
	0.4722000D+01	0.7871000D+01	0.1162000D+05	0.3924000D+03
	0.4402000D-02	0.2651000D-01	0.2065000D+04	-0.2007000D+02
	0.7426000D+01	-0.9899000D+00	0.5707000D-01	-0.1209000D-02
	0.6000000D+00	0.3605000D+01	0.4612000D+01	0.3181300D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
I	53.000			
	0.4748000D+01	0.8716000D+01	0.1183000D+05	0.3948000D+03
	0.4376000D-02	0.2702000D-01	0.2052000D+04	-0.2056000D+02
	0.7627000D+01	-0.1019000D+01	0.5896000D-01	-0.1254000D-02
	0.6190000D+00	0.4557000D+01	0.4852000D+01	0.3316900D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
XE	54.000			
	0.4589000D+01	0.9289000D+01	0.1203000D+05	0.3973000D+03
	0.4384000D-02	0.2753000D-01	0.2056000D+04	-0.2106000D+02
	0.7828000D+01	-0.1049000D+01	0.6085000D-01	-0.1298000D-02
	0.7000000D+00	0.4781000D+01	0.5100000D+01	0.3458200D+02
	0.2440000D+01	0.2620000D+01	0.2700000D+01	0.3470000D+01
	0.2820000D+01	0.2880000D+01	0.2730000D-04	0.8030000D-03
	0.1030000D-02			
CS	55.000			
	0.4533000D+01	0.8218000D+01	0.1223000D+05	0.3997000D+03
	0.4447000D-02	0.2804000D-01	0.2086000D+04	-0.2040000D+02
	0.7540000D+01	-0.1004000D+01	0.5782000D-01	-0.1224000D-02
	0.7260000D+00	0.5011000D+01	0.5358000D+01	0.3595900D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2880000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
BA	56.000			
	0.4387000D+01	0.8911000D+01	0.1243000D+05	0.4021000D+03
	0.4511000D-02	0.2855000D-01	0.2116000D+04	-0.1974000D+02
	0.7252000D+01	-0.9588000D+00	0.5479000D-01	-0.1151000D-02
	0.7810000D+00	0.5247000D+01	0.5624000D+01	0.3744100D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2880000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
LA	57.000			
	0.4337000D+01	0.9071000D+01	0.1263000D+05	0.4045000D+03
	0.4540000D-02	0.2906000D-01	0.2129000D+04	-0.1908000D+02
	0.6964000D+01	-0.9136000D+00	0.5176000D-01	-0.1077000D-02
	0.8510000D+00	0.5483000D+01	0.5891000D+01	0.3892500D+02

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	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
CE	58.000			
	0.4300000D+01	0.8444000D+01	0.1283000D+05	0.4069000D+03
	0.4420000D-02	0.2957000D-01	0.2073000D+04	-0.1843000D+02
	0.6677000D+01	-0.8684000D+00	0.4872000D-01	-0.1003000D-02
	0.8830000D+00	0.5724000D+01	0.6165000D+01	0.4044900D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
PR	59.000			
	0.4276000D+01	0.8219000D+01	0.1303000D+05	0.4093000D+03
	0.4298000D-02	0.3008000D-01	0.2016000D+04	-0.1777000D+02
	0.6389000D+01	-0.8233000D+00	0.4569000D-01	-0.9292000D-03
	0.9510000D+00	0.5968000D+01	0.6443000D+01	0.4199800D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
ND	60.000			
	0.4177000D+01	0.8000000D+01	0.1323000D+05	0.4118000D+03
	0.4182000D-02	0.3059000D-01	0.1962000D+04	-0.1711000D+02
	0.6101000D+01	-0.7781000D+00	0.4266000D-01	-0.8553000D-03
	0.9780000D+00	0.6208000D+01	0.6722000D+01	0.4357100D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
PM	61.000			
	0.4099000D+01	0.7786000D+01	0.1343000D+05	0.4142000D+03
	0.4058000D-02	0.3110000D-01	0.1903000D+04	-0.1645000D+02
	0.5813000D+01	-0.7330000D+00	0.3963000D-01	-0.7815000D-03
	0.1052000D+01	0.6466000D+01	0.7018000D+01	0.4520700D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
SM	62.000			
	0.4007000D+01	0.7580000D+01	0.1362000D+05	0.4166000D+03
	0.3976000D-02	0.3161000D-01	0.1865000D+04	-0.1579000D+02
	0.5526000D+01	-0.6878000D+00	0.3660000D-01	-0.7077000D-03
	0.1108000D+01	0.6717000D+01	0.7312000D+01	0.4683500D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
EU	63.000			
	0.3965000D+01	0.7380000D+01	0.1382000D+05	0.4190000D+03
	0.3877000D-02	0.3212000D-01	0.1819000D+04	-0.1513000D+02
	0.5238000D+01	-0.6426000D+00	0.3357000D-01	-0.6339000D-03
	0.1611000D+01	0.6983000D+01	0.7624000D+01	0.4851500D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
GD	64.000			
	0.3831000D+01	0.7592000D+01	0.1402000D+05	0.4214000D+03
	0.3863000D-02	0.3263000D-01	0.1812000D+04	-0.1447000D+02
	0.4950000D+01	-0.5975000D+00	0.3053000D-01	-0.5601000D-03
	0.1221000D+01	0.7243000D+01	0.7931000D+01	0.5024000D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
TB	65.000			
	0.3791000D+01	0.6996000D+01	0.1421000D+05	0.4239000D+03
	0.3725000D-02	0.3314000D-01	0.1747000D+04	-0.1456000D+02
	0.4984000D+01	-0.6022000D+00	0.3082000D-01	-0.5668000D-03
	0.1280000D+01	0.7515000D+01	0.8252000D+01	0.5199600D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03

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	0.1240000D-02			
DY	66.000			
	0.3708000D+01	0.6210000D+01	0.1440000D+05	0.4263000D+03
	0.3632000D-02	0.3365000D-01	0.1703000D+04	-0.1465000D+02
	0.5018000D+01	-0.6069000D+00	0.3111000D-01	-0.5734000D-03
	0.1295000D+01	0.7850000D+01	0.8621000D+01	0.5378900D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
H0	67.000			
	0.3653000D+01	0.5874000D+01	0.1460000D+05	0.4287000D+03
	0.3498000D-02	0.3416000D-01	0.1640000D+04	-0.1474000D+02
	0.5051000D+01	-0.6117000D+00	0.3141000D-01	-0.5801000D-03
	0.1390000D+01	0.8071000D+01	0.8919000D+01	0.5561500D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
ER	68.000			
	0.3602000D+01	0.5706000D+01	0.1479000D+05	0.4330000D+03
	0.3405000D-02	0.3467000D-01	0.1597000D+04	-0.1483000D+02
	0.5085000D+01	-0.6164000D+00	0.3170000D-01	-0.5867000D-03
	0.1450000D+01	0.8364000D+01	0.9263000D+01	0.5748300D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
TM	69.000			
	0.3567000D+01	0.5542000D+01	0.1498000D+05	0.4335000D+03
	0.3342000D-02	0.3518000D-01	0.1567000D+04	-0.1491000D+02
	0.5119000D+01	-0.6211000D+00	0.3199000D-01	-0.5933000D-03
	0.1515000D+01	0.8648000D+01	0.9618000D+01	0.5939000D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
YB	70.000			
	0.3482000D+01	0.5386000D+01	0.1517000D+05	0.4359000D+03
	0.3292000D-02	0.3569000D-01	0.1544000D+04	-0.1500000D+02
	0.5153000D+01	-0.6258000D+00	0.3228000D-01	-0.6000000D-03
	0.1578000D+01	0.8943000D+01	0.9978000D+01	0.6133200D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
LU	71.000			
	0.3443000D+01	0.5505000D+01	0.1536000D+05	0.4384000D+03
	0.3243000D-02	0.3620000D-01	0.1521000D+04	-0.1509000D+02
	0.5186000D+01	-0.6305000D+00	0.3257000D-01	-0.6066000D-03
	0.1639000D+01	0.9241000D+01	0.1034500D+02	0.6330400D+02
	0.2500000D+01	0.2620000D+01	0.2700000D+01	0.2980000D+01
	0.2820000D+01	0.2830000D+01	0.1580000D-03	0.8030000D-03
	0.1240000D-02			
HF	72.000			
	0.3376000D+01	0.5657000D+01	0.1555000D+05	0.4408000D+03
	0.3195000D-02	0.3671000D-01	0.1499000D+04	-0.1518000D+02
	0.5220000D+01	-0.6353000D+00	0.3286000D-01	-0.6133000D-03
	0.1718000D+01	0.9561000D+01	0.1073900D+02	0.6535100D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
TA	73.000			
	0.3330000D+01	0.5329000D+01	0.1574000D+05	0.4432000D+03
	0.3186000D-02	0.3722000D-01	0.1494000D+04	-0.1527000D+02
	0.5254000D+01	-0.6400000D+00	0.3315000D-01	-0.6199000D-03
	0.1793000D+01	0.9881000D+01	0.1113900D+02	0.6741400D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
W	74.000			

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	0.3277000D+01	0.5144000D+01	0.1593000D+05	0.4424000D+03
	0.3144000D-02	0.3773000D-01	0.1475000D+04	-0.1567000D+02
	0.5392000D+01	-0.6577000D+00	0.3418000D-01	-0.6426000D-03
	0.1809000D+01	0.1020400D+02	0.1154200D+02	0.6952400D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
RE	75.000			
	0.3236000D+01	0.5851000D+01	0.1612000D+05	0.4416000D+03
	0.3122000D-02	0.3824000D-01	0.1464000D+04	-0.1607000D+02
	0.5529000D+01	-0.6755000D+00	0.3521000D-01	-0.6654000D-03
	0.1948000D+01	0.1053100D+02	0.1195500D+02	0.7166100D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
OS	76.000			
	0.3168000D+01	0.5704000D+01	0.1630000D+05	0.4409000D+03
	0.3082000D-02	0.3875000D-01	0.1446000D+04	-0.1647000D+02
	0.5667000D+01	-0.6932000D+00	0.3624000D-01	-0.6881000D-03
	0.2013000D+01	0.1086900D+02	0.1238300D+02	0.7386000D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
IR	77.000			
	0.3135000D+01	0.5563000D+01	0.1649000D+05	0.4401000D+03
	0.2965000D-02	0.3926000D-01	0.1390000D+04	-0.1688000D+02
	0.5804000D+01	-0.7110000D+00	0.3727000D-01	-0.7109000D-03
	0.2116000D+01	0.1121500D+02	0.1282400D+02	0.7611200D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
PT	78.000			
	0.3088000D+01	0.5034000D+01	0.1667000D+05	0.4393000D+03
	0.2871000D-02	0.3977000D-01	0.1347000D+04	-0.1728000D+02
	0.5942000D+01	-0.7287000D+00	0.3830000D-01	-0.7336000D-03
	0.2202000D+01	0.1156400D+02	0.1327300D+02	0.7839500D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
AU	79.000			
	0.3059000D+01	0.5460000D+01	0.1832000D+05	0.4385000D+03
	0.2542000D-02	0.4028000D-01	0.1354000D+04	-0.1702000D+02
	0.5846000D+01	-0.7149000D+00	0.3740000D-01	-0.7114000D-03
	0.2206000D+01	0.1191800D+02	0.1373300D+02	0.8072300D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
HG	80.000			
	0.3004000D+01	0.4843000D+01	0.1704000D+05	0.4878000D+03
	0.2882000D-02	0.4079000D-01	0.1352000D+04	-0.1784000D+02
	0.6183000D+01	-0.7659000D+00	0.4076000D-01	-0.7925000D-03
	0.2385000D+01	0.1228400D+02	0.1420900D+02	0.6310300D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
TL	81.000			
	0.2948000D+01	0.5311000D+01	0.1722000D+05	0.5370000D+03
	0.2913000D-02	0.4130000D-01	0.1366000D+04	-0.1866000D+02
	0.6520000D+01	-0.8169000D+00	0.4411000D-01	-0.8737000D-03
	0.2485000D+01	0.1265700D+02	0.1469800D+02	0.8552800D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
PB	82.000			
	0.2908000D+01	0.5982000D+01	0.1740000D+05	0.5863000D+03
	0.2871000D-02	0.4181000D-01	0.1347000D+04	-0.1948000D+02

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	0.6857000D+01	-0.8678000D+00	0.4747000D-01	-0.9548000D-03
	0.2484000D+01	0.1303500D+02	0.1519800D+02	0.8800600D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
BI	83.000			
	0.2883000D+01	0.6700000D+01	0.1780000D+05	0.6770000D+03
	0.2660000D-02	0.4232000D-01	0.1336000D+04	-0.1955000D+02
	0.6871000D+01	-0.8686000D+00	0.4748000D-01	-0.9544000D-03
	0.2580000D+01	0.1348100D+02	0.1570800D+02	0.9052700D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
PO	84.000			
	0.2869000D+01	0.6928000D+01	0.1777000D+05	0.5863000D+03
	0.2812000D-02	0.4283000D-01	0.1319000D+04	-0.1962000D+02
	0.6884000D+01	-0.8694000D+00	0.4748000D-01	-0.9540000D-03
	0.2798000D+01	0.1381700D+02	0.1624400D+02	0.9311200D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
AT	85.000			
	0.2869000D+01	0.6979000D+01	0.1795000D+05	0.5863000D+03
	0.2776000D-02	0.4334000D-01	0.1302000D+04	-0.1969000D+02
	0.6898000D+01	-0.8702000D+00	0.4749000D-01	-0.9536000D-03
	0.2910000D+01	0.1421500D+02	0.1678400D+02	0.9574000D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
RN	86.000			
	0.2714000D+01	0.6954000D+01	0.1812000D+05	0.5863000D+03
	0.2748000D-02	0.4385000D-01	0.1289000D+04	-0.1976000D+02
	0.6912000D+01	-0.8710000D+00	0.4749000D-01	-0.9532000D-03
	0.3020000D+01	0.1461800D+02	0.1733700D+02	0.9841800D+02
	0.2550000D+01	0.2620000D+01	0.2500000D+01	0.3090000D+01
	0.2820000D+01	0.3380000D+01	0.9390000D-04	0.8030000D-03
	0.1030000D-03			
FR	87.000			
	0.2702000D+01	0.7820000D+01	0.1830000D+05	0.5863000D+03
	0.2737000D-02	0.4436000D-01	0.1284000D+04	-0.1983000D+02
	0.6926000D+01	-0.8718000D+00	0.4750000D-01	-0.9528000D-03
	0.3140000D+01	0.1502800D+02	0.1790400D+02	0.1011470D+03
	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03
	0.1030000D-03			
RA	88.000			
	0.2666000D+01	0.8448000D+01	0.1848000D+05	0.5863000D+03
	0.2727000D-02	0.4487000D-01	0.1279000D+04	-0.1990000D+02
	0.6940000D+01	-0.8726000D+00	0.4751000D-01	-0.9524000D-03
	0.3250000D+01	0.1544200D+02	0.1907800D+02	0.1039270D+03
	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03
	0.1030000D-03			
AC	89.000			
	0.2654000D+01	0.8609000D+01	0.1866000D+05	0.5863000D+03
	0.2697000D-02	0.4538000D-01	0.1265000D+04	-0.1997000D+02
	0.6953000D+01	-0.8733000D+00	0.4751000D-01	-0.9520000D-03
	0.3370000D+01	0.1586500D+02	0.1907800D+02	0.1067590D+03
	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03
	0.1030000D-03			
TH	90.000			
	0.2597000D+01	0.8679000D+01	0.1883000D+05	0.5863000D+03
	0.2641000D-02	0.4589000D-01	0.1239000D+04	-0.2004000D+02
	0.6967000D+01	-0.8741000D+00	0.4752000D-01	-0.9516000D-03
	0.3332000D+01	0.1630000D+02	0.1969200D+02	0.1096490D+03

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	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01		
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03		
	0.1030000D-03					
PA	91.000					
	0.2608000D+01	0.8336000D+01	0.1901000D+05	0.5863000D+03		
	0.2603000D-02	0.4640000D-01	0.1221000D+04	-0.2011000D+02		
	0.6981000D+01	-0.8749000D+00	0.4752000D-01	-0.9512000D-03		
	0.3610000D+01	0.1673100D+02	0.2031100D+02	0.1125810D+03		
	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01		
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03		
	0.1030000D-03					
U	92.000					
	0.2531000D+01	0.8204000D+01	0.1918000D+05	0.5863000D+03		
	0.2573000D-02	0.4691000D-01	0.1207000D+04	-0.2018000D+02		
	0.6995000D+01	-0.8757000D+00	0.4753000D-01	-0.9508000D-03		
	0.3552000D+01	0.1716700D+02	0.2094700D+02	0.1156030D+03		
	0.2630000D+01	0.2620000D+01	0.2500000D+01	0.4260000D+01		
	0.2820000D+01	0.2380000D+01	0.5760000D-06	0.8030000D-03		
	0.1030000D-03					

Listing of dset4 data file

B	0.19200	5.00000	1.00000	0.18500	10.81000	0.00170
C	0.28300	6.00000	1.00000	0.27700	12.00000	0.00280
N	0.39900	7.00000	1.00000	0.39200	14.00000	0.00520
O	0.53100	8.00000	1.00000	0.52500	16.00000	0.00830
NA	1.07200	11.00000	1.00000	1.04100	23.00000	0.02300
MG	1.30500	12.00000	0.98717	1.25300	24.31200	0.03000
AL	1.55900	13.00000	0.98039	1.48600	26.98000	0.03900
SI	1.83900	14.00000	0.97371	1.74000	28.06500	0.05000
P	2.14200	15.00000	0.95877	2.01300	30.97000	0.06300
S	2.47200	16.00000	0.94429	2.30700	32.06400	0.07800
CL	2.82200	17.00000	0.92421	2.62200	35.45000	0.09700
AR	3.20200	18.00000	0.90498	2.95700	39.98000	0.11800
K	3.60700	19.00000	0.89526	3.31300	39.10000	0.14000
CA	4.03800	20.00000	0.88652	3.69100	40.08000	0.16300
SC	4.49600	21.00000	0.88417	4.09000	44.95600	0.18800
TI	4.96500	22.00000	0.88183	4.51000	47.90000	0.21400
V	5.46500	23.00000	0.88106	4.95000	50.94000	0.24300
CR	5.98900	24.00000	0.88106	5.41400	52.00000	0.27500
MN	6.54000	25.00000	0.88106	5.89600	54.94000	0.30800
FE	7.11200	26.00000	0.88106	6.40300	55.84000	0.34000
CO	7.70900	27.00000	0.88106	6.92900	58.93000	0.37300
NI	8.33300	28.00000	0.88106	7.47700	58.71000	0.40600
CU	8.97900	29.00000	0.87951	8.04600	63.54000	0.44000
ZN	9.65900	30.00000	0.87873	8.63700	65.37000	0.47400
GA	10.36800	31.00000	0.87489	9.25000	69.72000	0.50700
GE	11.10400	32.00000	0.87184	9.88500	72.59000	0.53500
AS	11.86800	33.00000	0.86806	10.54200	74.92000	0.56200
SE	12.65800	34.00000	0.86430	11.22000	78.96000	0.58900
BR	13.47400	35.00000	0.85543	11.92200	80.00000	0.61800
RB	15.20100	37.00000	0.84962	13.39300	85.47000	0.66700
SR	16.10500	38.00000	0.84746	14.10000	87.62000	0.69000
Y	17.03700	39.00000	0.84388	14.96000	88.91000	0.71000
ZR	17.99800	40.00000	0.84034	15.77200	91.22000	0.73000
NB	18.98600	41.00000	0.83752	16.61200	92.91000	0.74700
MO	20.00200	42.00000	0.83542	17.47600	95.94000	0.76500
TC	21.05400	43.00000	0.83260	18.36400	97.00000	0.77950
RU	22.11800	44.00000	0.83056	19.27600	101.07000	0.79400
RH	23.22400	45.00000	0.82850	20.21300	102.90000	0.80800
PD	24.35000	46.00000	0.82645	21.12100	106.40000	0.82000
AG	25.51400	47.00000	0.82508	22.15900	107.90000	0.83100
CD	26.71100	48.00000	0.82440	23.17000	112.40000	0.84300
IN	27.94000	49.00000	0.82237	24.20600	114.82000	0.85300
SN	29.20000	50.00000	0.81967	25.26700	119.00000	0.86200
SB	30.49100	51.00000	0.78490	26.35500	121.75000	0.87000

A.3 PIXAN data files

TE	31.81300	52.00000	0.81633	27.37700	127.60000	0.87700
I	33.16900	53.00000	0.81367	28.60700	126.90500	0.88400
CS	35.95900	55.00000	0.81037	30.85100	132.91000	0.89600
BA	37.44100	56.00000	0.80800	32.18800	137.34000	0.90200
LA	38.92500	57.00000	0.80645	33.29900	138.91000	0.90700
CE	40.44900	58.00000	0.80515	34.56600	140.12000	0.91200
PR	41.99800	59.00000	0.80360	36.02000	140.90800	0.91600
ND	43.57100	60.00000	0.80240	37.35500	144.24100	0.92100
SM	46.83500	62.00000	0.80000	39.91100	150.40000	0.92900
ZRL	2.32500	40.00000	0.64558	2.04200	91.22000	0.03095
NBL	2.47625	41.00000	0.64226	2.16600	92.91000	0.03354
MOL	2.63275	42.00000	0.63980	2.29300	95.94000	0.03633
TCL	2.80075	43.00000	0.63012	2.42400	97.00000	0.03931
RUL	2.96900	44.00000	0.61881	2.55800	101.07000	0.04249
RHL	3.14275	45.00000	0.61087	2.69600	102.91000	0.04589
PDL	3.32325	46.00000	0.60350	2.83800	106.40000	0.04952
AGL	3.50800	47.00000	0.59312	2.98400	107.87000	0.05338
CDL	3.70500	48.00000	0.58309	3.13300	112.40000	0.05748
INL	3.90875	49.00000	0.54945	3.28600	114.82000	0.06184
SNL	4.11975	50.00000	0.51975	3.44300	118.69000	0.06646
SBL	4.33575	51.00000	0.51975	3.60400	121.75000	0.07135
TEL	4.55825	52.00000	0.51975	3.76900	127.60000	0.07653
IL	4.78850	53.00000	0.52110	3.93700	126.90000	0.08199
XEL	5.02850	54.00000	0.52247	4.10900	131.30000	0.08775
CSL	5.27500	55.00000	0.52138	4.28600	132.91000	0.09381
BAL	5.52825	56.00000	0.52056	4.46500	137.34000	0.10018
LAL	5.78100	57.00000	0.52356	4.65000	138.91000	0.10687
CEL	6.04050	58.00000	0.52604	4.83900	140.12000	0.11388
PRL	6.30625	59.00000	0.52938	5.03300	140.91000	0.12121
NDL	6.56600	60.00000	0.53248	5.22900	144.24000	0.12886
PML	6.84950	61.00000	0.53533	5.43200	145.00000	0.13684
SML	7.12075	62.00000	0.53792	5.63500	150.40000	0.14516
EUL	7.41475	63.00000	0.54113	5.84500	151.96000	0.15379
GDL	7.69825	64.00000	0.54407	6.05600	157.25000	0.16276
TBL	7.99750	65.00000	0.54705	6.27200	158.93000	0.17204
DYL	8.35100	66.00000	0.55006	6.49400	162.50000	0.18164
HOL	8.61400	67.00000	0.55402	6.71900	164.93000	0.19155
ERL	8.94175	68.00000	0.55772	6.94700	167.26000	0.20176
TML	9.25750	69.00000	0.56117	7.17900	168.93000	0.21227
YBL	9.61250	70.00000	0.56465	7.41400	173.04000	0.22306
LUL	9.92350	71.00000	0.56338	7.65400	174.97000	0.23412
HFL	10.28125	72.00000	0.56211	7.89800	178.49000	0.24545
TAL	10.64525	73.00000	0.56370	8.14500	180.95000	0.25701
WL	11.01200	74.00000	0.56433	8.39600	183.85000	0.26881
REL	11.38475	75.00000	0.57013	8.65100	186.21000	0.28082
OSL	11.77150	76.00000	0.57604	8.91000	190.20000	0.29302
IRL	12.16950	77.00000	0.58072	9.17400	192.22000	0.30541
PTL	12.57325	78.00000	0.58514	9.44100	195.09000	0.31795
AUL	12.98050	79.00000	0.58824	9.71200	196.97000	0.33063
HGL	13.40575	80.00000	0.59067	9.98700	200.59000	0.34343
TLL	13.83900	81.00000	0.59242	10.26700	204.37000	0.35633
PBL	14.28200	82.00000	0.59453	10.55000	207.20000	0.36931
BIL	14.73225	83.00000	0.59559	10.83700	208.98000	0.38235
POL	15.20325	84.00000	0.59666	11.12900	209.00000	0.39542
ATL	15.67600	85.00000	0.59737	11.42500	210.00000	0.40851
RNL	16.15775	86.00000	0.59809	11.72500	222.00000	0.42160
FRL	16.64950	87.00000	0.60680	12.02900	223.00000	0.43467
RAL	17.29875	88.00000	0.61576	12.33800	226.03000	0.44769
ACL	17.66250	89.00000	0.60976	12.65000	227.00000	0.46066
THL	18.19050	90.00000	0.60386	12.96700	232.04000	0.47354
PAL	18.71875	91.00000	0.60976	13.28800	231.04000	0.48633
UL	19.25925	92.00000	0.61538	13.61200	238.03000	0.49901

Listing of dset5 data file

-1ENER

A PIXAN PACKAGE

89				
0.6000000D+01	0.5900000D+01	0.5800000D+01	0.5700000D+01	
0.5600000D+01	0.5500000D+01	0.5400000D+01	0.5300000D+01	
0.5200000D+01	0.5100000D+01	0.5000000D+01	0.4900000D+01	
0.4800000D+01	0.4700000D+01	0.4600000D+01	0.4500000D+01	
0.4400000D+01	0.4300000D+01	0.4200000D+01	0.4100000D+01	
0.4000000D+01	0.3900000D+01	0.3800000D+01	0.3700000D+01	
0.3600000D+01	0.3500000D+01	0.3400000D+01	0.3300000D+01	
0.3200000D+01	0.3100000D+01	0.3000000D+01	0.2950000D+01	
0.2900000D+01	0.2850000D+01	0.2800000D+01	0.2750000D+01	
0.2700000D+01	0.2650000D+01	0.2600000D+01	0.2550000D+01	
0.2500000D+01	0.2450000D+01	0.2400000D+01	0.2350000D+01	
0.2300000D+01	0.2250000D+01	0.2200000D+01	0.2150000D+01	
0.2100000D+01	0.2050000D+01	0.2000000D+01	0.1950000D+01	
0.1900000D+01	0.1850000D+01	0.1800000D+01	0.1750000D+01	
0.1700000D+01	0.1650000D+01	0.1600000D+01	0.1550000D+01	
0.1500000D+01	0.1450000D+01	0.1400000D+01	0.1350000D+01	
0.1300000D+01	0.1250000D+01	0.1200000D+01	0.1150000D+01	
0.1100000D+01	0.1050000D+01	0.1000000D+01	0.9500000D+00	
0.9000000D+00	0.8500000D+00	0.8000000D+00	0.7500000D+00	
0.7000000D+00	0.6500000D+00	0.6000000D+00	0.5500000D+00	
0.5000000D+00	0.4500000D+00	0.4000000D+00	0.3500000D+00	
0.3000000D+00	0.2500000D+00	0.2000000D+00	0.1500000D+00	
0.1000000D+00				
6C				
89				
0.3295011D+06	0.3335799D+06	0.3377712D+06	0.3420797D+06	
0.3465105D+06	0.3510689D+06	0.3557607D+06	0.3605919D+06	
0.3655690D+06	0.3706987D+06	0.3759883D+06	0.3814456D+06	
0.3870787D+06	0.3928963D+06	0.3989079D+06	0.4051234D+06	
0.4115533D+06	0.4182092D+06	0.4251031D+06	0.4322481D+06	
0.4396581D+06	0.4473483D+06	0.4553346D+06	0.4636345D+06	
0.4722664D+06	0.4812453D+06	0.4906036D+06	0.5003587D+06	
0.5105359D+06	0.5211619D+06	0.5322660D+06	0.5380070D+06	
0.5438795D+06	0.5498876D+06	0.5560360D+06	0.5623291D+06	
0.5687718D+06	0.5753690D+06	0.5821258D+06	0.5890474D+06	
0.5961394D+06	0.6034073D+06	0.6108569D+06	0.6184941D+06	
0.6263250D+06	0.6343557D+06	0.6425925D+06	0.6510418D+06	
0.6597100D+06	0.6686036D+06	0.6777287D+06	0.6870917D+06	
0.6966986D+06	0.7065551D+06	0.7166663D+06	0.7270369D+06	
0.7376707D+06	0.7485703D+06	0.7597370D+06	0.7711703D+06	
0.7828673D+06	0.7948223D+06	0.8070258D+06	0.8194637D+06	
0.8321160D+06	0.8449555D+06	0.8579453D+06	0.8710369D+06	
0.8841671D+06	0.8972531D+06	0.9101885D+06	0.9228354D+06	
0.9350160D+06	0.9465007D+06	0.9569921D+06	0.9661042D+06	
0.9733330D+06	0.9780169D+06	0.9792823D+06	0.9759650D+06	
0.9665019D+06	0.9487733D+06	0.9198812D+06	0.8758366D+06	
0.8111560D+06	0.7184230D+06	0.5885781D+06	0.4136892D+06	
0.2023802D+06				
7N				
89				
0.2094526D+06	0.2119134D+06	0.2144375D+06	0.2170274D+06	
0.2196857D+06	0.2224152D+06	0.2252188D+06	0.2280994D+06	
0.2310602D+06	0.2341046D+06	0.2372362D+06	0.2404564D+06	
0.2437737D+06	0.2471899D+06	0.2507094D+06	0.2543367D+06	
0.2580767D+06	0.2619345D+06	0.2659154D+06	0.2700251D+06	
0.2742695D+06	0.2786550D+06	0.2831881D+06	0.2878756D+06	
0.2927249D+06	0.2977434D+06	0.3029390D+06	0.3083199D+06	
0.3138944D+06	0.3196712D+06	0.3256591D+06	0.3287349D+06	
0.3318668D+06	0.3350558D+06	0.3383030D+06	0.3416095D+06	
0.3449762D+06	0.3484040D+06	0.3518940D+06	0.3554469D+06	
0.3590634D+06	0.3627443D+06	0.3664899D+06	0.3703007D+06	
0.3741768D+06	0.3781182D+06	0.3821245D+06	0.3861951D+06	
0.3903291D+06	0.3945249D+06	0.3987808D+06	0.4030941D+06	
0.4074617D+06	0.4118796D+06	0.4163427D+06	0.4208449D+06	
0.4253788D+06	0.4299353D+06	0.4345036D+06	0.4390705D+06	

A.3 PIXAN data files

0.4436204D+06	0.4481344D+06	0.4525902D+06	0.4569609D+06
0.4612144D+06	0.4653126D+06	0.4692094D+06	0.4728501D+06
0.4761688D+06	0.4790862D+06	0.4815067D+06	0.4833149D+06
0.4843707D+06	0.4845035D+06	0.4835051D+06	0.4811198D+06
0.4770327D+06	0.4708543D+06	0.4621002D+06	0.4501670D+06
0.4343014D+06	0.4135643D+06	0.3867763D+06	0.3525847D+06
0.3093762D+06	0.2556291D+06	0.1907186D+06	0.1172810D+06
0.4683699D+05			
80			
89			
0.1425397D+06	0.1441025D+06	0.1457018D+06	0.1473389D+06
0.1490151D+06	0.1507315D+06	0.1524898D+06	0.1542912D+06
0.1561372D+06	0.1580295D+06	0.1599696D+06	0.1619591D+06
0.1639998D+06	0.1660934D+06	0.1682418D+06	0.1704468D+06
0.1727103D+06	0.1750343D+06	0.1774208D+06	0.1798717D+06
0.1823891D+06	0.1849751D+06	0.1876315D+06	0.1903605D+06
0.1931637D+06	0.1960430D+06	0.1989999D+06	0.2020357D+06
0.2051515D+06	0.2083479D+06	0.2116248D+06	0.2132934D+06
0.2149817D+06	0.2166897D+06	0.2184171D+06	0.2201633D+06
0.2219281D+06	0.2237108D+06	0.2255107D+06	0.2273270D+06
0.2291588D+06	0.2310050D+06	0.2328641D+06	0.2347348D+06
0.2366153D+06	0.2385034D+06	0.2403970D+06	0.2422933D+06
0.2441892D+06	0.2460813D+06	0.2479655D+06	0.2498373D+06
0.2516914D+06	0.2535220D+06	0.2553220D+06	0.2570838D+06
0.2587987D+06	0.2604563D+06	0.2620452D+06	0.2635520D+06
0.2649618D+06	0.2662570D+06	0.2674178D+06	0.2684212D+06
0.2692409D+06	0.2698464D+06	0.2702026D+06	0.2702688D+06
0.2699980D+06	0.2693352D+06	0.2682165D+06	0.2665674D+06
0.2643004D+06	0.2613131D+06	0.2574850D+06	0.2526743D+06
0.2467135D+06	0.2394057D+06	0.2305195D+06	0.2197732D+06
0.2068796D+06	0.1914749D+06	0.1731857D+06	0.1516577D+06
0.1266591D+06	0.9831125D+05	0.6757681D+05	0.3718133D+05
0.1274638D+05			
9F			
89			
0.9936683D+05	0.1003667D+06	0.1013870D+06	0.1024281D+06
0.1034906D+06	0.1045750D+06	0.1056820D+06	0.1068120D+06
0.1079656D+06	0.1091433D+06	0.1103458D+06	0.1115734D+06
0.1128268D+06	0.1141065D+06	0.1154129D+06	0.1167464D+06
0.1181076D+06	0.1194966D+06	0.1209139D+06	0.1223595D+06
0.1238336D+06	0.1253361D+06	0.1268669D+06	0.1284255D+06
0.1300114D+06	0.1316238D+06	0.1332613D+06	0.1349224D+06
0.1366050D+06	0.1383066D+06	0.1400237D+06	0.1408869D+06
0.1417523D+06	0.1426194D+06	0.1434872D+06	0.1443552D+06
0.1452222D+06	0.1460872D+06	0.1469492D+06	0.1478069D+06
0.1486589D+06	0.1495036D+06	0.1503394D+06	0.1511644D+06
0.1519764D+06	0.1527732D+06	0.1535522D+06	0.1543106D+06
0.1550452D+06	0.1557526D+06	0.1564289D+06	0.1570698D+06
0.1576706D+06	0.1582259D+06	0.1587299D+06	0.1591761D+06
0.1595572D+06	0.1598649D+06	0.1600903D+06	0.1602232D+06
0.1602522D+06	0.1601646D+06	0.1599462D+06	0.1595808D+06
0.1590505D+06	0.1583349D+06	0.1574112D+06	0.1562534D+06
0.1548324D+06	0.1531151D+06	0.1510639D+06	0.1486364D+06
0.1457845D+06	0.1424536D+06	0.1385820D+06	0.1340937D+06
0.1289253D+06	0.1229827D+06	0.1161723D+06	0.1083948D+06
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0.7081091D+05	0.7145098D+05	0.7210164D+05	0.7276302D+05
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0.7623468D+05	0.7696250D+05	0.7770154D+05	0.7845178D+05
0.7921314D+05	0.7998550D+05	0.8076868D+05	0.8156244D+05
0.8236646D+05	0.8318034D+05	0.8400358D+05	0.8483556D+05
0.8567552D+05	0.8652258D+05	0.8737563D+05	0.8823338D+05

A PIXAN PACKAGE

0.8909430D+05	0.8995657D+05	0.9081805D+05	0.9167622D+05
0.9252809D+05	0.9337018D+05	0.9419840D+05	0.9460583D+05
0.9500793D+05	0.9540395D+05	0.9579311D+05	0.9617454D+05
0.9654732D+05	0.9691041D+05	0.9726273D+05	0.9760307D+05
0.9793015D+05	0.9824255D+05	0.9853875D+05	0.9881707D+05
0.9907572D+05	0.9931272D+05	0.9952593D+05	0.9971301D+05
0.9987142D+05	0.9999838D+05	0.1000909D+06	0.1001456D+06
0.1001589D+06	0.1001268D+06	0.1000451D+06	0.9990893D+05
0.9971313D+05	0.9945202D+05	0.9911932D+05	0.9870815D+05
0.9821095D+05	0.9761938D+05	0.9692427D+05	0.9611554D+05
0.9518204D+05	0.9411148D+05	0.9289032D+05	0.9150358D+05
0.8993484D+05	0.8816594D+05	0.8617251D+05	0.8394205D+05
0.8144579D+05	0.7865785D+05	0.7555054D+05	0.7209446D+05
0.6825929D+05	0.6401477D+05	0.5933278D+05	0.5419050D+05
0.4857574D+05	0.4249560D+05	0.3599014D+05	0.2915352D+05
0.2216535D+05	0.1533254D+05	0.9130749D+04	0.4198738D+04
0.1157749D+04			
11NA			
89			
0.5133040D+05	0.5173608D+05	0.5214649D+05	0.5256157D+05
0.5298124D+05	0.5340540D+05	0.5383391D+05	0.5426663D+05
0.5470338D+05	0.5514394D+05	0.5558806D+05	0.5603545D+05
0.5648578D+05	0.5693863D+05	0.5739358D+05	0.5785008D+05
0.5830755D+05	0.5876530D+05	0.5922255D+05	0.5967841D+05
0.6013186D+05	0.6058174D+05	0.6102673D+05	0.6146533D+05
0.6189582D+05	0.6231625D+05	0.6272440D+05	0.6311772D+05
0.6349334D+05	0.6384795D+05	0.6417778D+05	0.6433208D+05
0.6447852D+05	0.6461647D+05	0.6474523D+05	0.6486409D+05
0.6497226D+05	0.6506889D+05	0.6515310D+05	0.6522391D+05
0.6528029D+05	0.6532113D+05	0.6534524D+05	0.6535133D+05
0.6533802D+05	0.6530383D+05	0.6524716D+05	0.6516631D+05
0.6505941D+05	0.6492448D+05	0.6475937D+05	0.6456176D+05
0.6432914D+05	0.6405882D+05	0.6374787D+05	0.6339316D+05
0.6299128D+05	0.6253854D+05	0.6203096D+05	0.6146423D+05
0.6083368D+05	0.6013430D+05	0.5936063D+05	0.5850677D+05
0.5756638D+05	0.5652986D+05	0.5539558D+05	0.5415262D+05
0.5279253D+05	0.5130635D+05	0.4968457D+05	0.4791727D+05
0.4599423D+05	0.4390513D+05	0.4163989D+05	0.3918913D+05
0.3654499D+05	0.3370222D+05	0.3065978D+05	0.2742336D+05
0.2400871D+05	0.2044670D+05	0.1679008D+05	0.1312224D+05
0.9567660D+04	0.6300321D+04	0.3541097D+04	0.1522813D+04
0.3891109D+03			
12MG			
89			
0.3761501D+05	0.3786579D+05	0.3811787D+05	0.3837110D+05
0.3862530D+05	0.3888027D+05	0.3913580D+05	0.3939164D+05
0.3964751D+05	0.3990310D+05	0.4015809D+05	0.4041208D+05
0.4066465D+05	0.4091534D+05	0.4116360D+05	0.4140886D+05
0.4165047D+05	0.4188769D+05	0.4211973D+05	0.4234567D+05
0.4256453D+05	0.4277517D+05	0.4297635D+05	0.4316668D+05
0.4334461D+05	0.4350840D+05	0.4365612D+05	0.4378557D+05
0.4389435D+05	0.4397972D+05	0.4403861D+05	0.4405707D+05
0.4406759D+05	0.4406968D+05	0.4406279D+05	0.4404638D+05
0.4401985D+05	0.4398257D+05	0.4393386D+05	0.4387302D+05
0.4379927D+05	0.4371183D+05	0.4360982D+05	0.4349233D+05
0.4335839D+05	0.4320697D+05	0.4303697D+05	0.4284720D+05
0.4263642D+05	0.4240329D+05	0.4214639D+05	0.4186421D+05
0.4155512D+05	0.4121741D+05	0.4084924D+05	0.4044866D+05
0.4001358D+05	0.3954178D+05	0.3903089D+05	0.3847664D+05
0.3788004D+05	0.3723637D+05	0.3654262D+05	0.3579567D+05
0.3499220D+05	0.3412875D+05	0.3320172D+05	0.3220742D+05
0.3114205D+05	0.3000183D+05	0.2878303D+05	0.2748208D+05
0.2609580D+05	0.2462152D+05	0.2305748D+05	0.2140319D+05
0.1966004D+05	0.1783202D+05	0.1592685D+05	0.1395720D+05
0.1194263D+05	0.9911647D+04	0.7904359D+04	0.5974971D+04
0.4193353D+04	0.2643305D+04	0.1413570D+04	0.5746800D+03

A.3 PIXAN data files

0.1376639D+03			
13AL			
89			
0.2804603D+05	0.2819626D+05	0.2834591D+05	0.2849480D+05
0.2864271D+05	0.2878942D+05	0.2893471D+05	0.2907830D+05
0.2921989D+05	0.2935919D+05	0.2949583D+05	0.2962944D+05
0.2975961D+05	0.2988587D+05	0.3000773D+05	0.3012465D+05
0.3023602D+05	0.3034119D+05	0.3043943D+05	0.3052995D+05
0.3061188D+05	0.3068427D+05	0.3074606D+05	0.3079609D+05
0.3083308D+05	0.3085564D+05	0.3086219D+05	0.3085104D+05
0.3082028D+05	0.3076783D+05	0.3069135D+05	0.3064331D+05
0.3058828D+05	0.3052590D+05	0.3045577D+05	0.3037750D+05
0.3029067D+05	0.3019481D+05	0.3008945D+05	0.2997410D+05
0.2984822D+05	0.2971127D+05	0.2956265D+05	0.2940174D+05
0.2922790D+05	0.2904044D+05	0.2883863D+05	0.2862170D+05
0.2838886D+05	0.2813925D+05	0.2787196D+05	0.2758608D+05
0.2727935D+05	0.2695330D+05	0.2660551D+05	0.2623482D+05
0.2584005D+05	0.2541992D+05	0.2497314D+05	0.2449831D+05
0.2399404D+05	0.2345886D+05	0.2289127D+05	0.2228974D+05
0.2165274D+05	0.2097872D+05	0.2026617D+05	0.1951367D+05
0.1871987D+05	0.1788361D+05	0.1700399D+05	0.1608041D+05
0.1511281D+05	0.1410172D+05	0.1304855D+05	0.1195585D+05
0.1082764D+05	0.9669898D+04	0.8491012D+04	0.7302536D+04
0.6119802D+04	0.4962799D+04	0.3856685D+04	0.2832073D+04
0.1924118D+04	0.1169615D+04	0.6006289D+03	0.2332829D+03
0.5281874D+02			
14SI			
89			
0.2111320D+05	0.2119744D+05	0.2128013D+05	0.2136110D+05
0.2144015D+05	0.2151708D+05	0.2159164D+05	0.2166360D+05
0.2173269D+05	0.2179862D+05	0.2186108D+05	0.2191973D+05
0.2197421D+05	0.2202411D+05	0.2206902D+05	0.2210845D+05
0.2214192D+05	0.2216886D+05	0.2218868D+05	0.2220073D+05
0.2220432D+05	0.2219867D+05	0.2218296D+05	0.2215626D+05
0.2211760D+05	0.2206589D+05	0.2199995D+05	0.2191851D+05
0.2182016D+05	0.2170337D+05	0.2156646D+05	0.2148989D+05
0.2140760D+05	0.2131931D+05	0.2122478D+05	0.2112371D+05
0.2101581D+05	0.2090078D+05	0.2077830D+05	0.2064803D+05
0.2050962D+05	0.2036271D+05	0.2020690D+05	0.2004181D+05
0.1986611D+05	0.1968122D+05	0.1948573D+05	0.1927918D+05
0.1906105D+05	0.1883085D+05	0.1858804D+05	0.1833207D+05
0.1806235D+05	0.1777831D+05	0.1747932D+05	0.1716476D+05
0.1683398D+05	0.1648633D+05	0.1612114D+05	0.1573774D+05
0.1533546D+05	0.1491363D+05	0.1447163D+05	0.1400883D+05
0.1352465D+05	0.1301862D+05	0.1249030D+05	0.1193939D+05
0.1136578D+05	0.1076951D+05	0.1015089D+05	0.9510599D+04
0.8849692D+04	0.8169752D+04	0.7473045D+04	0.6762612D+04
0.6042489D+04	0.5317942D+04	0.4595633D+04	0.3883938D+04
0.3193088D+04	0.2535376D+04	0.1925022D+04	0.1377805D+04
0.9099571D+03	0.5361202D+03	0.2659176D+03	0.9928931D+02
0.2128791D+02			
15P			
89			
0.1602377D+05	0.1606517D+05	0.1610463D+05	0.1614199D+05
0.1617707D+05	0.1620970D+05	0.1623967D+05	0.1626676D+05
0.1629076D+05	0.1631141D+05	0.1632846D+05	0.1634162D+05
0.1635058D+05	0.1635503D+05	0.1635462D+05	0.1634896D+05
0.1633765D+05	0.1632027D+05	0.1629633D+05	0.1626533D+05
0.1622674D+05	0.1617996D+05	0.1612437D+05	0.1605927D+05
0.1598394D+05	0.1589758D+05	0.1579934D+05	0.1568828D+05
0.1556341D+05	0.1542366D+05	0.1526785D+05	0.1518354D+05
0.1509472D+05	0.1500125D+05	0.1490294D+05	0.1479959D+05
0.1469037D+05	0.1457640D+05	0.1445679D+05	0.1433134D+05
0.1419982D+05	0.1406199D+05	0.1391763D+05	0.1376648D+05
0.1360828D+05	0.1344278D+05	0.1326971D+05	0.1308879D+05
0.1289972D+05	0.1270223D+05	0.1249602D+05	0.1228077D+05

A PIXAN PACKAGE

0.1205619D+05	0.1182196D+05	0.1157778D+05	0.1132333D+05
0.1105832D+05	0.1078243D+05	0.1049539D+05	0.1019692D+05
0.9886785D+04	0.9564751D+04	0.9230635D+04	0.8884314D+04
0.8525709D+04	0.8154824D+04	0.7771751D+04	0.7376715D+04
0.6970068D+04	0.6552339D+04	0.6124263D+04	0.5686848D+04
0.5241391D+04	0.4789548D+04	0.4333435D+04	0.3875651D+04
0.3419384D+04	0.2968516D+04	0.2527647D+04	0.2102207D+04
0.1698407D+04	0.1323220D+04	0.9841115D+03	0.6886519D+03
0.4437462D+03	0.2544633D+03	0.1224503D+03	0.4410294D+02
0.8964815D+01			
16S			
89			
0.1223748D+05	0.1225157D+05	0.1226364D+05	0.1227357D+05
0.1228120D+05	0.1228638D+05	0.1228896D+05	0.1228874D+05
0.1228556D+05	0.1227920D+05	0.1226946D+05	0.1225612D+05
0.1223892D+05	0.1221762D+05	0.1219194D+05	0.1216159D+05
0.1212626D+05	0.1208561D+05	0.1203930D+05	0.1198694D+05
0.1192812D+05	0.1186241D+05	0.1178935D+05	0.1170845D+05
0.1161918D+05	0.1152096D+05	0.1141320D+05	0.1129526D+05
0.1116644D+05	0.1102554D+05	0.1087276D+05	0.1079146D+05
0.1070675D+05	0.1061852D+05	0.1052664D+05	0.1043100D+05
0.1033148D+05	0.1022796D+05	0.1012030D+05	0.1000837D+05
0.9892037D+04	0.9771165D+04	0.9645611D+04	0.9515234D+04
0.9379885D+04	0.9239417D+04	0.9093682D+04	0.8942528D+04
0.8785802D+04	0.8623358D+04	0.8455045D+04	0.8280714D+04
0.8100220D+04	0.7913431D+04	0.7720211D+04	0.7520439D+04
0.7314003D+04	0.7100804D+04	0.6880773D+04	0.6653848D+04
0.6420003D+04	0.6179236D+04	0.5931602D+04	0.5677186D+04
0.5416138D+04	0.5148671D+04	0.4875076D+04	0.4595751D+04
0.4311190D+04	0.4022019D+04	0.3729011D+04	0.3433131D+04
0.3135525D+04	0.2837571D+04	0.2540924D+04	0.2247512D+04
0.1959578D+04	0.1679724D+04	0.1410870D+04	0.1156289D+04
0.9195120D+03	0.7042497D+03	0.5141881D+03	0.3526927D+03
0.2223719D+03	0.1244938D+03	0.5831742D+02	0.2028490D+02
0.3902725D+01			
17CL			
89			
0.9432840D+04	0.9430191D+04	0.9425638D+04	0.9419068D+04
0.9410364D+04	0.9399401D+04	0.9386050D+04	0.9370171D+04
0.9351616D+04	0.9330228D+04	0.9305844D+04	0.9278288D+04
0.9247375D+04	0.9212909D+04	0.9174680D+04	0.9132471D+04
0.9086046D+04	0.9035160D+04	0.8979548D+04	0.8918933D+04
0.8853020D+04	0.8781497D+04	0.8704036D+04	0.8620285D+04
0.8529517D+04	0.8432078D+04	0.8327172D+04	0.8214367D+04
0.8093201D+04	0.7963189D+04	0.7823829D+04	0.7750476D+04
0.7674585D+04	0.7596085D+04	0.7514905D+04	0.7430974D+04
0.7344216D+04	0.7254556D+04	0.7161921D+04	0.7066233D+04
0.6967414D+04	0.6865386D+04	0.6760075D+04	0.6651400D+04
0.6539286D+04	0.6423656D+04	0.6304434D+04	0.6181551D+04
0.6054935D+04	0.5924520D+04	0.5790245D+04	0.5652048D+04
0.5509886D+04	0.5363714D+04	0.5213498D+04	0.5059216D+04
0.4900860D+04	0.4738434D+04	0.4571970D+04	0.4401511D+04
0.4227130D+04	0.4048928D+04	0.3867035D+04	0.3681633D+04
0.3492938D+04	0.3301220D+04	0.3106805D+04	0.2910101D+04
0.2711580D+04	0.2511803D+04	0.2311431D+04	0.2111244D+04
0.1912134D+04	0.1715132D+04	0.1521409D+04	0.1332301D+04
0.1149286D+04	0.9740081D+03	0.8082358D+03	0.6538557D+03
0.5127928D+03	0.3869428D+03	0.2780339D+03	0.1874453D+03
0.1159799D+03	0.6358270D+02	0.2906245D+02	0.9785164D+01
0.1780377D+01			
18AR			
89			
0.7285826D+04	0.7273240D+04	0.7258944D+04	0.7242849D+04
0.7224863D+04	0.7204888D+04	0.7182822D+04	0.7158557D+04
0.7131982D+04	0.7102976D+04	0.7071414D+04	0.7037163D+04
0.7000086D+04	0.6960035D+04	0.6916856D+04	0.6870389D+04

A.3 PIXAN data files

0.6820464D+04	0.6766900D+04	0.6709509D+04	0.6647825D+04
0.6582191D+04	0.6512109D+04	0.6437348D+04	0.6357668D+04
0.6272819D+04	0.6182541D+04	0.6086559D+04	0.5984591D+04
0.5876341D+04	0.5761507D+04	0.5639774D+04	0.5576220D+04
0.5510821D+04	0.5443535D+04	0.5374322D+04	0.5303141D+04
0.5229949D+04	0.5154707D+04	0.5077373D+04	0.4997906D+04
0.4916269D+04	0.4832423D+04	0.4746329D+04	0.4657954D+04
0.4567261D+04	0.4474219D+04	0.4378803D+04	0.4280984D+04
0.4180742D+04	0.4078058D+04	0.3972921D+04	0.3865323D+04
0.3755269D+04	0.3642766D+04	0.3527832D+04	0.3410497D+04
0.3290801D+04	0.3168797D+04	0.3044560D+04	0.2918177D+04
0.2789757D+04	0.2659431D+04	0.2527354D+04	0.2393720D+04
0.2258746D+04	0.2122688D+04	0.1985845D+04	0.1848556D+04
0.1711224D+04	0.1574294D+04	0.1438276D+04	0.1303742D+04
0.1171344D+04	0.1041793D+04	0.9158776D+03	0.7944655D+03
0.6784794D+03	0.5689087D+03	0.4667700D+03	0.3730945D+03
0.2888767D+03	0.2150176D+03	0.1522471D+03	0.1010262D+03
0.6142955D+02	0.3303468D+02	0.1473690D+02	0.4801637D+01
0.8228725D+00			
19K			
89			
0.5655006D+04	0.5637085D+04	0.5617680D+04	0.5596723D+04
0.5574142D+04	0.5549865D+04	0.5523812D+04	0.5495903D+04
0.5466052D+04	0.5434171D+04	0.5400166D+04	0.5363940D+04
0.5325392D+04	0.5284198D+04	0.5240689D+04	0.5194525D+04
0.5145582D+04	0.5093735D+04	0.5038853D+04	0.4980798D+04
0.4919428D+04	0.4854595D+04	0.4786147D+04	0.4713923D+04
0.4637762D+04	0.4557493D+04	0.4472946D+04	0.4383943D+04
0.4290303D+04	0.4191849D+04	0.4088396D+04	0.4034738D+04
0.3979764D+04	0.3923452D+04	0.3865780D+04	0.3806727D+04
0.3746272D+04	0.3684396D+04	0.3621080D+04	0.3556308D+04
0.3490063D+04	0.3422330D+04	0.3353096D+04	0.3282351D+04
0.3210086D+04	0.3136292D+04	0.3060972D+04	0.2984124D+04
0.2905751D+04	0.2825863D+04	0.2744474D+04	0.2661603D+04
0.2577273D+04	0.2491522D+04	0.2404388D+04	0.2315921D+04
0.2226179D+04	0.2135234D+04	0.2043166D+04	0.1950077D+04
0.1856075D+04	0.1761290D+04	0.1665868D+04	0.1569978D+04
0.1473807D+04	0.1377574D+04	0.1281520D+04	0.1185913D+04
0.1091054D+04	0.9972815D+03	0.9049614D+03	0.8144984D+03
0.7263305D+03	0.6409382D+03	0.5588256D+03	0.4805343D+03
0.4066194D+03	0.3376532D+03	0.2741976D+03	0.2167937D+03
0.1659245D+03	0.1219845D+03	0.8523394D+02	0.5574751D+02
0.3337075D+02	0.1760835D+02	0.7673881D+01	0.2417450D+01
0.3882456D+00			
20CA			
89			
0.4406561D+04	0.4386278D+04	0.4364739D+04	0.4341894D+04
0.4317689D+04	0.4292067D+04	0.4264972D+04	0.4236172D+04
0.4205952D+04	0.4174070D+04	0.4140459D+04	0.4105048D+04
0.4067765D+04	0.4028532D+04	0.3987274D+04	0.3943908D+04
0.3898350D+04	0.3850514D+04	0.3800310D+04	0.3747648D+04
0.3692432D+04	0.3634565D+04	0.3573950D+04	0.3510483D+04
0.3444065D+04	0.3374593D+04	0.3301961D+04	0.3226068D+04
0.3146813D+04	0.3064097D+04	0.2977825D+04	0.2933326D+04
0.2887907D+04	0.2841557D+04	0.2794266D+04	0.2746027D+04
0.2696832D+04	0.2646675D+04	0.2595549D+04	0.2543450D+04
0.2490379D+04	0.2436333D+04	0.2381312D+04	0.2325320D+04
0.2268362D+04	0.2210445D+04	0.2151580D+04	0.2091779D+04
0.2031062D+04	0.1969449D+04	0.1906964D+04	0.1843638D+04
0.1779505D+04	0.1714606D+04	0.1648985D+04	0.1582701D+04
0.1515813D+04	0.1448390D+04	0.1380510D+04	0.1312263D+04
0.1243745D+04	0.1175071D+04	0.1106363D+04	0.1037759D+04
0.9694080D+03	0.9014770D+03	0.8341534D+03	0.7676358D+03
0.7021428D+03	0.6379093D+03	0.5751947D+03	0.5142697D+03
0.4554227D+03	0.3989615D+03	0.3451995D+03	0.2944629D+03
0.2470743D+03	0.2033523D+03	0.1635954D+03	0.1280699D+03

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0.9699254D+02	0.7050968D+02	0.4867319D+02	0.3142494D+02
0.1852588D+02	0.9602600D+01	0.4090005D+01	0.1244716D+01
0.1865079D+00			
21SC			
89			
0.3444720D+04	0.3423963D+04	0.3402164D+04	0.3379285D+04
0.3355285D+04	0.3330126D+04	0.3303763D+04	0.3276153D+04
0.3247253D+04	0.3217014D+04	0.3185390D+04	0.3152330D+04
0.3117785D+04	0.3081701D+04	0.3044025D+04	0.3004702D+04
0.2963677D+04	0.2920892D+04	0.2876287D+04	0.2829805D+04
0.2781386D+04	0.2730968D+04	0.2678490D+04	0.2623895D+04
0.2567122D+04	0.2508112D+04	0.2446809D+04	0.2383159D+04
0.2317114D+04	0.2248627D+04	0.2177660D+04	0.2141236D+04
0.2104180D+04	0.2066492D+04	0.2028169D+04	0.1989210D+04
0.1949616D+04	0.1909387D+04	0.1868526D+04	0.1827036D+04
0.1784922D+04	0.1742189D+04	0.1698848D+04	0.1654908D+04
0.1610380D+04	0.1565277D+04	0.1519617D+04	0.1473418D+04
0.1426702D+04	0.1379492D+04	0.1331820D+04	0.1283715D+04
0.1235213D+04	0.1186355D+04	0.1137184D+04	0.1087751D+04
0.1038110D+04	0.9883244D+03	0.9384603D+03	0.8885918D+03
0.8388001D+03	0.7891745D+03	0.7398103D+03	0.6908168D+03
0.6423070D+03	0.5944048D+03	0.5472420D+03	0.5009653D+03
0.4557254D+03	0.4116844D+03	0.3690117D+03	0.3278883D+03
0.2884966D+03	0.2510278D+03	0.2156706D+03	0.1826147D+03
0.1520416D+03	0.1241202D+03	0.9899977D+02	0.7680119D+02
0.5760646D+02	0.4144733D+02	0.2829265D+02	0.1804262D+02
0.1048604D+02	0.5342558D+01	0.2224383D+01	0.6532808D+00
0.9092086D-01			
22TI			
89			
0.2719347D+04	0.2699243D+04	0.2678284D+04	0.2656442D+04
0.2633687D+04	0.2609991D+04	0.2585323D+04	0.2559652D+04
0.2532947D+04	0.2505174D+04	0.2476301D+04	0.2446293D+04
0.2415115D+04	0.2382733D+04	0.2349109D+04	0.2314210D+04
0.2277997D+04	0.2240433D+04	0.2201482D+04	0.2161109D+04
0.2119275D+04	0.2075945D+04	0.2031085D+04	0.1984661D+04
0.1936642D+04	0.1886999D+04	0.1835705D+04	0.1782738D+04
0.1728077D+04	0.1671713D+04	0.1613638D+04	0.1583959D+04
0.1553854D+04	0.1523324D+04	0.1492372D+04	0.1460999D+04
0.1429213D+04	0.1397017D+04	0.1364416D+04	0.1331418D+04
0.1298032D+04	0.1264265D+04	0.1230130D+04	0.1195639D+04
0.1160804D+04	0.1125643D+04	0.1090174D+04	0.1054415D+04
0.1018388D+04	0.9821171D+03	0.9456296D+03	0.9089547D+03
0.8721232D+03	0.8351537D+03	0.7981436D+03	0.7610752D+03
0.7240149D+03	0.6870129D+03	0.6501223D+03	0.6134052D+03
0.5769240D+03	0.5407472D+03	0.5049486D+03	0.4696059D+03
0.4348062D+03	0.7006378D+03	0.3671955D+03	0.3345783D+03
0.3028933D+03	0.2722484D+03	0.2427554D+03	0.2145314D+03
0.1876915D+03	0.1623527D+03	0.1386285D+03	0.1166273D+03
0.9644900D+02	0.7818142D+02	0.6189533D+02	0.4763929D+02
0.3543369D+02	0.2526429D+02	0.1708167D+02	0.1076869D+02
0.6177343D+01	0.3096675D+01	0.1260888D+01	0.3571620D+00
0.4597675D-01			
23V			
89			
0.2148069D+04	0.2129260D+04	0.2109759D+04	0.2089545D+04
0.2068598D+04	0.2046897D+04	0.2024421D+04	0.2001149D+04
0.1977058D+04	0.1952127D+04	0.1926334D+04	0.1899655D+04
0.1872068D+04	0.1843549D+04	0.1814077D+04	0.1783628D+04
0.1752181D+04	0.1719713D+04	0.1686202D+04	0.1651627D+04
0.1615970D+04	0.1579211D+04	0.1541333D+04	0.1502321D+04
0.1462161D+04	0.1420845D+04	0.1378363D+04	0.1334715D+04
0.1289899D+04	0.1243923D+04	0.1196800D+04	0.1172814D+04
0.1148550D+04	0.1124011D+04	0.1099202D+04	0.1074128D+04
0.1048795D+04	0.1023209D+04	0.9973781D+03	0.9713091D+03
0.9450139D+03	0.9185017D+03	0.8917837D+03	0.8648728D+03

A.3 PIXAN data files

0.8377828D+03	0.8105288D+03	0.7831276D+03	0.7555975D+03
0.7279570D+03	0.7002303D+03	0.6724397D+03	0.6446104D+03
0.6167701D+03	0.5889485D+03	0.5611776D+03	0.5334908D+03
0.5059276D+03	0.4785264D+03	0.4513298D+03	0.4243830D+03
0.3977333D+03	0.3714342D+03	0.3455390D+03	0.3201047D+03
0.2951918D+03	0.2708622D+03	0.2471837D+03	0.2242233D+03
0.2020505D+03	0.1807381D+03	0.1603573D+03	0.1409814D+03
0.1226815D+03	0.1055265D+03	0.8958157D+02	0.7490629D+02
0.6155232D+02	0.4956103D+02	0.3896063D+02	0.2976306D+02
0.2196057D+02	0.1552738D+02	0.1039460D+02	0.6481474D+01
0.3669951D+01	0.1809752D+01	0.7199132D+00	0.1961970D+00
0.2319243D-01			
24CR			
89			
0.1702788D+04	0.1685600D+04	0.1667856D+04	0.1649543D+04
0.1630646D+04	0.1611153D+04	0.1591047D+04	0.1570316D+04
0.1548943D+04	0.1526915D+04	0.1504218D+04	0.1480838D+04
0.1456759D+04	0.1431968D+04	0.1406452D+04	0.1380197D+04
0.1353191D+04	0.1325422D+04	0.1296879D+04	0.1267552D+04
0.1237430D+04	0.1206509D+04	0.1174782D+04	0.1142245D+04
0.1108897D+04	0.1074738D+04	0.1039773D+04	0.1004011D+04
0.9674647D+03	0.9301497D+03	0.8920891D+03	0.8727880D+03
0.8533119D+03	0.8336645D+03	0.8138532D+03	0.7938827D+03
0.7737594D+03	0.7534904D+03	0.7330834D+03	0.7125467D+03
0.6918895D+03	0.6711218D+03	0.6502543D+03	0.6292976D+03
0.6082668D+03	0.5871742D+03	0.5660346D+03	0.5448639D+03
0.5236792D+03	0.5024987D+03	0.4813420D+03	0.4602292D+03
0.4391848D+03	0.4182316D+03	0.3973951D+03	0.3767025D+03
0.3561824D+03	0.3358644D+03	0.3157827D+03	0.2959701D+03
0.2764624D+03	0.2572969D+03	0.2385119D+03	0.2201497D+03
0.2022517D+03	0.1848613D+03	0.1680227D+03	0.1517824D+03
0.1361854D+03	0.1212785D+03	0.1071070D+03	0.9371528D+02
0.8114595D+02	0.6943882D+02	0.5862987D+02	0.4875000D+02
0.3982369D+02	0.3186739D+02	0.2488785D+02	0.1888029D+02
0.1383073D+02	0.9696310D+01	0.6431526D+01	0.3967968D+01
0.2218106D+01	0.1075753D+01	0.4177652D+00	0.1092799D+00
0.1177661D-01			
25MN			
89			
0.1352909D+04	0.1337466D+04	0.1321583D+04	0.1305249D+04
0.1288456D+04	0.1271195D+04	0.1253455D+04	0.1235228D+04
0.1216505D+04	0.1197277D+04	0.1177534D+04	0.1157270D+04
0.1136475D+04	0.1115142D+04	0.1093265D+04	0.1070835D+04
0.1047847D+04	0.1024297D+04	0.1000181D+04	0.9754947D+03
0.9502370D+03	0.9244076D+03	0.8980079D+03	0.8710404D+03
0.8435123D+03	0.8154308D+03	0.7868066D+03	0.7576540D+03
0.7279907D+03	0.6978376D+03	0.6672229D+03	0.6517519D+03
0.6361777D+03	0.6205050D+03	0.6047394D+03	0.5888864D+03
0.5729523D+03	0.5569438D+03	0.5408671D+03	0.5247320D+03
0.5085457D+03	0.4923172D+03	0.4760561D+03	0.4597725D+03
0.4434775D+03	0.4271826D+03	0.4109004D+03	0.3946431D+03
0.3784267D+03	0.3622651D+03	0.3461742D+03	0.3301707D+03
0.3142725D+03	0.2984981D+03	0.2828665D+03	0.2674002D+03
0.2521200D+03	0.2370487D+03	0.2222103D+03	0.2076280D+03
0.1933313D+03	0.1793441D+03	0.1656946D+03	0.1524107D+03
0.1395223D+03	0.1270585D+03	0.1150485D+03	0.1035227D+03
0.9251062D+02	0.8204098D+02	0.7214182D+02	0.6283966D+02
0.5415907D+02	0.4612199D+02	0.3874704D+02	0.3204872D+02
0.2603656D+02	0.2071412D+02	0.1607803D+02	0.1212044D+02
0.8813257D+01	0.6130099D+01	0.4029998D+01	0.2460580D+01
0.1358029D+01	0.6475582D+00	0.2452810D+00	0.6143630D-01
0.5992684D-02			
26FE			
89			
0.1079564D+04	0.1065855D+04	0.1051799D+04	0.1037389D+04
0.1022620D+04	0.1007486D+04	0.9919823D+03	0.9761023D+03

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0.9598410D+03	0.9431934D+03	0.9261551D+03	0.9087215D+03
0.8908882D+03	0.8726530D+03	0.8540125D+03	0.8349644D+03
0.8155072D+03	0.7956404D+03	0.7753643D+03	0.7546794D+03
0.7335899D+03	0.7120990D+03	0.6902122D+03	0.6679368D+03
0.6452818D+03	0.6222589D+03	0.5988809D+03	0.5751661D+03
0.5511333D+03	0.5268055D+03	0.5022094D+03	0.4898204D+03
0.4773763D+03	0.4648809D+03	0.4523408D+03	0.4397605D+03
0.4271456D+03	0.4145020D+03	0.4018361D+03	0.3891548D+03
0.3764652D+03	0.3637751D+03	0.3510925D+03	0.3384252D+03
0.3257840D+03	0.3131776D+03	0.3006162D+03	0.2881106D+03
0.2756721D+03	0.2633124D+03	0.2510435D+03	0.2388797D+03
0.2268342D+03	0.2149212D+03	0.2031558D+03	0.1915534D+03
0.1801298D+03	0.1689029D+03	0.1578895D+03	0.1471075D+03
0.1365749D+03	0.1263114D+03	0.1163359D+03	0.1066674D+03
0.9732631D+02	0.8833174D+02	0.7970351D+02	0.7146071D+02
0.6362202D+02	0.5620533D+02	0.4922743D+02	0.4270372D+02
0.3664780D+02	0.3107105D+02	0.2598218D+02	0.2138674D+02
0.1728652D+02	0.1367902D+02	0.1055975D+02	0.7909496D+01
0.5712575D+01	0.3943649D+01	0.2570425D+01	0.1553496D+01
0.8465602D+00	0.3967571D+00	0.1464327D+00	0.3502646D-01
0.3067934D-02			
27CO			
89			
0.8638319D+03	0.8517745D+03	0.8394460D+03	0.8268429D+03
0.8139617D+03	0.8007991D+03	0.7873520D+03	0.7736177D+03
0.7595930D+03	0.7452767D+03	0.7306663D+03	0.7157603D+03
0.7005576D+03	0.6850575D+03	0.6692602D+03	0.6531661D+03
0.6367760D+03	0.6200931D+03	0.6031198D+03	0.5858601D+03
0.5683191D+03	0.5505029D+03	0.5324193D+03	0.5140768D+03
0.4954874D+03	0.4766631D+03	0.4576187D+03	0.4383710D+03
0.4189396D+03	0.3993459D+03	0.3796164D+03	0.3697092D+03
0.3597789D+03	0.3498295D+03	0.3398654D+03	0.3298912D+03
0.3199119D+03	0.3099325D+03	0.2999579D+03	0.2899951D+03
0.2800496D+03	0.2701276D+03	0.2602360D+03	0.2503816D+03
0.2405720D+03	0.2308149D+03	0.2211184D+03	0.2114904D+03
0.2019409D+03	0.1924787D+03	0.1831134D+03	0.1738550D+03
0.1647139D+03	0.1557004D+03	0.1468268D+03	0.1381041D+03
0.1295441D+03	0.1211590D+03	0.1129611D+03	0.1049637D+03
0.9717943D+02	0.8962119D+02	0.8230253D+02	0.7523663D+02
0.6843649D+02	0.6191502D+02	0.5568485D+02	0.4975814D+02
0.4414641D+02	0.3886041D+02	0.3390988D+02	0.2930329D+02
0.2504767D+02	0.2114825D+02	0.1760818D+02	0.1442826D+02
0.1160912D+02	0.9140402D+01	0.7016191D+01	0.5224419D+01
0.3748946D+01	0.2569320D+01	0.1660637D+01	0.9935652D+00
0.5345081D+00	0.2461245D+00	0.8841572D-01	0.2014329D-01
0.1571986D-02			
28NI			
89			
0.6926502D+03	0.6821246D+03	0.6713893D+03	0.6604422D+03
0.6492823D+03	0.6379076D+03	0.6263170D+03	0.6145094D+03
0.6024840D+03	0.5902404D+03	0.5777784D+03	0.5650984D+03
0.5522006D+03	0.5390872D+03	0.5257593D+03	0.5122193D+03
0.4984701D+03	0.4845154D+03	0.4703597D+03	0.4560075D+03
0.4414665D+03	0.4267433D+03	0.4118463D+03	0.3967853D+03
0.3815715D+03	0.3662174D+03	0.3507367D+03	0.3351468D+03
0.3194650D+03	0.3037117D+03	0.2879093D+03	0.2799974D+03
0.2720828D+03	0.2641692D+03	0.2562596D+03	0.2483591D+03
0.2404713D+03	0.2326004D+03	0.2247511D+03	0.2169280D+03
0.2091362D+03	0.2013807D+03	0.1936671D+03	0.1860003D+03
0.1783874D+03	0.1708340D+03	0.1633464D+03	0.1559312D+03
0.1485953D+03	0.1413458D+03	0.1341896D+03	0.1271352D+03
0.1201898D+03	0.1133616D+03	0.1066587D+03	0.1000893D+03
0.9366263D+02	0.8738704D+02	0.8127121D+02	0.7532452D+02
0.6955562D+02	0.6397369D+02	0.5858755D+02	0.5340601D+02
0.4843766D+02	0.4369083D+02	0.3917350D+02	0.3489315D+02
0.3085668D+02	0.2707027D+02	0.2353924D+02	0.2026790D+02

A.3 PIXAN data files

0.1725937D+02	0.1451539D+02	0.1203617D+02	0.9822291D+01
0.7865733D+01	0.6162964D+01	0.4705988D+01	0.3484246D+01
0.2484462D+01	0.1690533D+01	0.1083509D+01	0.6416912D+00
0.3406525D+00	0.1539898D+00	0.5375202D-01	0.1161981D-01
0.8002876D-03			
29CU			
89			
0.5573953D+03	0.5482543D+03	0.5389525D+03	0.5294893D+03
0.5198642D+03	0.5100769D+03	0.5001273D+03	0.4900151D+03
0.4797416D+03	0.4693070D+03	0.4587126D+03	0.4479595D+03
0.4370498D+03	0.4259855D+03	0.4147694D+03	0.4034047D+03
0.3918948D+03	0.3802450D+03	0.3684599D+03	0.3565454D+03
0.3445081D+03	0.3323555D+03	0.3200961D+03	0.3077389D+03
0.2952956D+03	0.2827774D+03	0.2701976D+03	0.2575707D+03
0.2449129D+03	0.2322419D+03	0.2195768D+03	0.2132535D+03
0.2069400D+03	0.2006393D+03	0.1943544D+03	0.1880887D+03
0.1818456D+03	0.1756285D+03	0.1694412D+03	0.1632871D+03
0.1571711D+03	0.1510969D+03	0.1450687D+03	0.1390910D+03
0.1331684D+03	0.1273057D+03	0.1215074D+03	0.1157795D+03
0.1101266D+03	0.1045543D+03	0.9906799D+02	0.9367337D+02
0.8837592D+02	0.8318214D+02	0.7809771D+02	0.7312872D+02
0.6828114D+02	0.6356146D+02	0.5897585D+02	0.5453046D+02
0.5023144D+02	0.4608486D+02	0.4209670D+02	0.3827274D+02
0.3461853D+02	0.3113934D+02	0.2784009D+02	0.2472525D+02
0.2179878D+02	0.1906406D+02	0.1652373D+02	0.1417965D+02
0.1203274D+02	0.1008291D+02	0.8330729D+01	0.6769833D+01
0.5398146D+01	0.4210239D+01	0.3199031D+01	0.2355694D+01
0.1669580D+01	0.1128184D+01	0.7171741D+00	0.4204310D+00
0.2202419D+00	0.9770198D-01	0.3310683D-01	0.6774401D-02
0.4083959D-03			
30ZN			
89			
0.4485615D+03	0.4406682D+03	0.4326533D+03	0.4245167D+03
0.4162593D+03	0.4078813D+03	0.3993833D+03	0.3907664D+03
0.3820316D+03	0.3731804D+03	0.3642145D+03	0.3551361D+03
0.3459470D+03	0.3366511D+03	0.3272509D+03	0.3177502D+03
0.3081532D+03	0.2984644D+03	0.2886892D+03	0.2788333D+03
0.2689029D+03	0.2589061D+03	0.2488504D+03	0.2387447D+03
0.2285987D+03	0.2184231D+03	0.2082296D+03	0.1980306D+03
0.1878410D+03	0.1776755D+03	0.1675506D+03	0.1625089D+03
0.1574843D+03	0.1524791D+03	0.1474959D+03	0.1425370D+03
0.1376059D+03	0.1327051D+03	0.1278375D+03	0.1230062D+03
0.1182144D+03	0.1134653D+03	0.1087622D+03	0.1041084D+03
0.9950791D+02	0.9496422D+02	0.9048102D+02	0.8606216D+02
0.8171158D+02	0.7743304D+02	0.7323114D+02	0.6910978D+02
0.6507319D+02	0.6112546D+02	0.5727123D+02	0.5351459D+02
0.4986002D+02	0.4631175D+02	0.4287407D+02	0.3955122D+02
0.3634734D+02	0.3326646D+02	0.3031246D+02	0.2748905D+02
0.2479971D+02	0.2224765D+02	0.1983575D+02	0.1756654D+02
0.1544211D+02	0.1346406D+02	0.1163346D+02	0.9950717D+01
0.8415565D+01	0.7028501D+01	0.5784420D+01	0.4682111D+01
0.3717794D+01	0.2886614D+01	0.2182581D+01	0.1598520D+01
0.1126043D+01	0.7555484D+00	0.4762791D+00	0.2762643D+00
0.1427108D+00	0.6205373D-01	0.2036712D-01	0.3926374D-02
0.2045508D-03			
31GA			
89			
0.3615755D+03	0.3547872D+03	0.3479084D+03	0.3409395D+03
0.3338815D+03	0.3267352D+03	0.3195020D+03	0.3121831D+03
0.3047798D+03	0.2972947D+03	0.2897294D+03	0.2820864D+03
0.2743684D+03	0.2665784D+03	0.2587197D+03	0.2507960D+03
0.2428115D+03	0.2347705D+03	0.2266787D+03	0.2185413D+03
0.2103643D+03	0.2021545D+03	0.1939191D+03	0.1856660D+03
0.1774035D+03	0.1691418D+03	0.1608905D+03	0.1526607D+03
0.1444643D+03	0.1363139D+03	0.1282230D+03	0.1242047D+03
0.1202069D+03	0.1162317D+03	0.1122812D+03	0.1083573D+03

A PIXAN PACKAGE

0.1044624D+03	0.1005988D+03	0.9676861D+02	0.9297411D+02
0.8921832D+02	0.8550346D+02	0.8183212D+02	0.7820696D+02
0.7463069D+02	0.7110586D+02	0.6763576D+02	0.6422303D+02
0.6087059D+02	0.5758140D+02	0.5435832D+02	0.5120466D+02
0.4812326D+02	0.4511728D+02	0.4218971D+02	0.3934360D+02
0.3658195D+02	0.3390772D+02	0.3132384D+02	0.2883312D+02
0.2643831D+02	0.2414203D+02	0.2194673D+02	0.1985473D+02
0.1786812D+02	0.1598876D+02	0.1421826D+02	0.1255789D+02
0.1100861D+02	0.9570993D+01	0.8245157D+01	0.7032113D+01
0.5928253D+01	0.4933475D+01	0.4045757D+01	0.3262412D+01
0.2580042D+01	0.1994502D+01	0.1500867D+01	0.1093410D+01
0.7655957D+00	0.5101010D+00	0.3188239D+00	0.1829539D+00
0.9315691D-01	0.3967059D-01	0.1259057D-01	0.2278168D-02
0.1014709D-03			
32GE			
89			
0.2921141D+03	0.2862937D+03	0.2804067D+03	0.2744542D+03
0.2684370D+03	0.2623569D+03	0.2562150D+03	0.2500130D+03
0.2437527D+03	0.2374360D+03	0.2310652D+03	0.2246427D+03
0.2181713D+03	0.2116540D+03	0.2050937D+03	0.1984947D+03
0.1918606D+03	0.1851957D+03	0.1785047D+03	0.1717925D+03
0.1650648D+03	0.1583271D+03	0.1515866D+03	0.1448497D+03
0.1381241D+03	0.1314178D+03	0.1247392D+03	0.1180978D+03
0.1115031D+03	0.1049661D+03	0.9849793D+02	0.9529329D+02
0.9211036D+02	0.8895074D+02	0.8581606D+02	0.8270777D+02
0.7962812D+02	0.7657861D+02	0.7356108D+02	0.7057738D+02
0.6762940D+02	0.6471911D+02	0.6184827D+02	0.5901931D+02
0.5623407D+02	0.5349463D+02	0.5080297D+02	0.4816147D+02
0.4557216D+02	0.4303715D+02	0.4055871D+02	0.3813897D+02
0.3578009D+02	0.3348423D+02	0.3125353D+02	0.2909009D+02
0.2699597D+02	0.2497319D+02	0.2302368D+02	0.2114931D+02
0.1935185D+02	0.1763295D+02	0.1599412D+02	0.1443675D+02
0.1296204D+02	0.1157098D+02	0.1026437D+02	0.9042747D+01
0.7906386D+01	0.6855261D+01	0.5890165D+01	0.5008028D+01
0.4208922D+01	0.3491348D+01	0.2853361D+01	0.2292541D+01
0.1805967D+01	0.1390197D+01	0.1041252D+01	0.7546106D+00
0.5252106D+00	0.3474877D+00	0.2153069D+00	0.1221942D+00
0.6129488D-01	0.2553690D-01	0.7821270D-02	0.1322396D-02
0.4972543D-04			
33AS			
89			
0.2364698D+03	0.2314917D+03	0.2264657D+03	0.2213932D+03
0.2162752D+03	0.2111132D+03	0.2059087D+03	0.2006633D+03
0.1953790D+03	0.1900577D+03	0.1847013D+03	0.1793129D+03
0.1738947D+03	0.1684497D+03	0.1629808D+03	0.1574915D+03
0.1519853D+03	0.1464661D+03	0.1409378D+03	0.1354056D+03
0.1298739D+03	0.1243480D+03	0.1188335D+03	0.1133361D+03
0.1078625D+03	0.1024189D+03	0.9701322D+02	0.9165279D+02
0.8634573D+02	0.8110062D+02	0.7592628D+02	0.7336882D+02
0.7083274D+02	0.6831928D+02	0.6582976D+02	0.6336548D+02
0.6092781D+02	0.5851813D+02	0.5613766D+02	0.5378819D+02
0.5147100D+02	0.4918756D+02	0.4693937D+02	0.4472784D+02
0.4255471D+02	0.4042143D+02	0.3832950D+02	0.3628057D+02
0.34227617D+02	0.3231786D+02	0.3040718D+02	0.2854570D+02
0.2673494D+02	0.2497640D+02	0.2327156D+02	0.2162187D+02
0.2002870D+02	0.1849339D+02	0.1701723D+02	0.1560139D+02
0.1424699D+02	0.1295504D+02	0.1172643D+02	0.1056192D+02
0.9462155D+01	0.8427589D+01	0.7458519D+01	0.6555048D+01
0.5718066D+01	0.4945212D+01	0.4236887D+01	0.3592254D+01
0.3010188D+01	0.2489259D+01	0.2027714D+01	0.1623461D+01
0.1274055D+01	0.9766875D+00	0.7281822D+00	0.5249924D+00
0.3632282D+00	0.2385953D+00	0.1465389D+00	0.8222501D-01
0.4060830D-01	0.1653368D-01	0.4876248D-02	0.7668214D-02
0.2402201D-04			
34SE			
89			

A.3 PIXAN data files

0.1919118D+03	0.1876612D+03	0.1833773D+03	0.1790611D+03
0.1747139D+03	0.1703371D+03	0.1659321D+03	0.1615009D+03
0.1570451D+03	0.1525666D+03	0.1480675D+03	0.1435501D+03
0.1390168D+03	0.1344703D+03	0.1299132D+03	0.1253484D+03
0.1207797D+03	0.1162101D+03	0.1116435D+03	0.1070836D+03
0.1025347D+03	0.9800132D+02	0.9348809D+02	0.8899984D+02
0.8454238D+02	0.8012108D+02	0.7574189D+02	0.7141108D+02
0.6713504D+02	0.6292111D+02	0.5877631D+02	0.5673218D+02
0.5470820D+02	0.5270536D+02	0.5072450D+02	0.4876699D+02
0.4683369D+02	0.4492569D+02	0.4304404D+02	0.4118974D+02
0.3936411D+02	0.3756814D+02	0.3580292D+02	0.3406967D+02
0.3236948D+02	0.3070348D+02	0.2907282D+02	0.2747862D+02
0.2592202D+02	0.2440414D+02	0.2292608D+02	0.2148893D+02
0.2009375D+02	0.1874159D+02	0.1743345D+02	0.1617029D+02
0.1495304D+02	0.1378257D+02	0.1265968D+02	0.1158512D+02
0.1055955D+02	0.9583559D+01	0.8657631D+01	0.7782151D+01
0.6957386D+01	0.6183481D+01	0.5460440D+01	0.4788980D+01
0.4167039D+01	0.3595010D+01	0.3072239D+01	0.2597871D+01
0.2170840D+01	0.1789858D+01	0.1453405D+01	0.1159718D+01
0.9067844D+00	0.6923389D+00	0.5138610D+00	0.3685801D+00
0.2534934D+00	0.1653178D+00	0.1006290D+00	0.5580930D-01
0.2712176D-01	0.1078056D-01	0.3055630D-02	0.4449563D-03
0.1146418D-04			
35BR			
89			
0.1561421D+03	0.1525173D+03	0.1488698D+03	0.1452011D+03
0.1415123D+03	0.1378048D+03	0.1340800D+03	0.1303394D+03
0.1265847D+03	0.1228178D+03	0.1190405D+03	0.1152549D+03
0.1114630D+03	0.1076676D+03	0.1038709D+03	0.1000756D+03
0.9628459D+02	0.9250076D+02	0.8872734D+02	0.8496769D+02
0.8122518D+02	0.7750400D+02	0.7380792D+02	0.7014112D+02
0.6650802D+02	0.6291325D+02	0.5936148D+02	0.5585817D+02
0.5240844D+02	0.4901781D+02	0.4569188D+02	0.4405515D+02
0.4243688D+02	0.4083784D+02	0.3925881D+02	0.3770058D+02
0.3616388D+02	0.3464968D+02	0.3315873D+02	0.3169180D+02
0.3024980D+02	0.2883353D+02	0.2744382D+02	0.2608151D+02
0.2474743D+02	0.2344242D+02	0.2216730D+02	0.2092289D+02
0.1970999D+02	0.1852941D+02	0.1738190D+02	0.1626824D+02
0.1518915D+02	0.1414534D+02	0.1313748D+02	0.1216621D+02
0.1123212D+02	0.1033576D+02	0.9477630D+01	0.8658171D+01
0.7877756D+01	0.7136692D+01	0.6435207D+01	0.5773446D+01
0.5151462D+01	0.4569964D+01	0.4027272D+01	0.3523867D+01
0.3059366D+01	0.2633253D+01	0.2244873D+01	0.1893421D+01
0.1577939D+01	0.1297307D+01	0.1050235D+01	0.8352621D+00
0.6507497D+00	0.4948824D+00	0.3656681D+00	0.2609591D+00
0.1783838D+00	0.1154859D+00	0.6965241D-01	0.3816472D-01
0.1823671D-01	0.7067426D-02	0.1920306D-02	0.2577785D-03
0.5371872D-05			
36KR			
89			
0.1271824D+03	0.1240968D+03	0.1209969D+03	0.1178839D+03
0.1147589D+03	0.1116231D+03	0.1084779D+03	0.1053249D+03
0.1021654D+03	0.9900086D+02	0.9583353D+02	0.9266498D+02
0.8949716D+02	0.8633213D+02	0.8317208D+02	0.8001931D+02
0.7687627D+02	0.7374533D+02	0.7062961D+02	0.6753175D+02
0.6445475D+02	0.6140178D+02	0.5837613D+02	0.5538126D+02
0.5242063D+02	0.4949833D+02	0.4661814D+02	0.4378412D+02
0.4100040D+02	0.3827159D+02	0.3560208D+02	0.3429100D+02
0.3299641D+02	0.3171908D+02	0.3045951D+02	0.2921827D+02
0.2799607D+02	0.2679346D+02	0.2561106D+02	0.2444950D+02
0.2330940D+02	0.2219137D+02	0.2109602D+02	0.2002397D+02
0.1897583D+02	0.1795220D+02	0.1695367D+02	0.1598082D+02
0.1503422D+02	0.1411442D+02	0.1322195D+02	0.1235735D+02
0.1152109D+02	0.1071365D+02	0.9935464D+01	0.9186938D+01
0.8468443D+01	0.7780309D+01	0.7122822D+01	0.6496220D+01
0.5900690D+01	0.5336361D+01	0.4803298D+01	0.4302161D+01

A PIXAN PACKAGE

0.3831551D+01	0.3391968D+01	0.2983183D+01	0.2604882D+01
0.2256654D+01	0.1937993D+01	0.1648285D+01	0.1386809D+01
0.1152728D+01	0.9450901D+00	0.7628201D+00	0.6047201D+00
0.4694671D+00	0.3556143D+00	0.2615929D+00	0.1857235D+00
0.1261806D+00	0.8108152D-01	0.4844174D-01	0.2621197D-01
0.1230667D-01	0.4644028D-02	0.1206737D-02	0.1484223D-03
0.2465723D-05			
37RB			
89			
0.1037459D+03	0.1011226D+03	0.9849129D+02	0.9585283D+02
0.9320834D+02	0.9055881D+02	0.8790582D+02	0.8525049D+02
0.8259417D+02	0.7993833D+02	0.7728448D+02	0.7463424D+02
0.7198932D+02	0.6935149D+02	0.6672247D+02	0.6410460D+02
0.6149977D+02	0.5891017D+02	0.5633807D+02	0.5378588D+02
0.5125608D+02	0.4875115D+02	0.4627409D+02	0.4382759D+02
0.4141457D+02	0.3903809D+02	0.3670119D+02	0.3440734D+02
0.3215977D+02	0.2996184D+02	0.2781723D+02	0.2676596D+02
0.2572939D+02	0.2470793D+02	0.2370203D+02	0.2271217D+02
0.2173879D+02	0.2078237D+02	0.1984336D+02	0.1892222D+02
0.1801941D+02	0.1713538D+02	0.1627058D+02	0.1542545D+02
0.1460044D+02	0.1379596D+02	0.1301245D+02	0.1225030D+02
0.1150991D+02	0.1079166D+02	0.1009591D+02	0.9423018D+01
0.8773295D+01	0.8147044D+01	0.7544543D+01	0.6966038D+01
0.6411746D+01	0.5881850D+01	0.5376498D+01	0.4895797D+01
0.4439812D+01	0.4009139D+01	0.3602593D+01	0.3220653D+01
0.2863184D+01	0.2529992D+01	0.2220816D+01	0.1935330D+01
0.1673137D+01	0.1433766D+01	0.1216668D+01	0.1021212D+01
0.8466857D+00	0.6922901D+00	0.5571394D+00	0.4402592D+00
0.3405871D+00	0.2569737D+00	0.1881952D+00	0.1329065D+00
0.8973375D-01	0.5721945D-01	0.3385143D-01	0.1807853D-01
0.8332160D-02	0.3056768D-02	0.7573736D-03	0.8481001D-04
0.1102524D-05			
38SR			
89			
0.8487113D+02	0.8264121D+02	0.8040747D+02	0.7817116D+02
0.7593311D+02	0.7369434D+02	0.7145595D+02	0.6921907D+02
0.6698493D+02	0.6475478D+02	0.6252997D+02	0.6031172D+02
0.5810184D+02	0.5590168D+02	0.5371286D+02	0.5153706D+02
0.4937603D+02	0.4723161D+02	0.4510556D+02	0.4300015D+02
0.4091730D+02	0.3885915D+02	0.3682792D+02	0.3482591D+02
0.3285539D+02	0.3091900D+02	0.2901915D+02	0.2715834D+02
0.2533935D+02	0.2356475D+02	0.2183732D+02	0.2099215D+02
0.2015980D+02	0.1934061D+02	0.1853494D+02	0.1774313D+02
0.1696552D+02	0.1620247D+02	0.1545430D+02	0.1472137D+02
0.1400400D+02	0.1330253D+02	0.1261728D+02	0.1194857D+02
0.1129670D+02	0.1066200D+02	0.1004473D+02	0.9445198D+01
0.8863660D+01	0.8300375D+01	0.7755585D+01	0.7229514D+01
0.6722368D+01	0.6234333D+01	0.5765575D+01	0.5316233D+01
0.4886423D+01	0.4476234D+01	0.4085723D+01	0.3714916D+01
0.3364313D+01	0.3032842D+01	0.2720929D+01	0.2428452D+01
0.2155244D+01	0.1901093D+01	0.1665738D+01	0.1448867D+01
0.1250113D+01	0.1069054D+01	0.9052125D+00	0.7580477D+00
0.6269598D+00	0.5112860D+00	0.4103005D+00	0.3232142D+00
0.2491755D+00	0.1872742D+00	0.1365338D+00	0.9591639D-01
0.6435082D-01	0.4071316D-01	0.2384443D-01	0.1256265D-01
0.5679273D-02	0.2022812D-02	0.4766549D-03	0.4831643D-04
0.4830492D-06			
39Y			
89			
0.6958320D+02	0.6768820D+02	0.6579274D+02	0.6389765D+02
0.6200380D+02	0.6011211D+02	0.5822354D+02	0.5633909D+02
0.5445967D+02	0.5258666D+02	0.5072108D+02	0.4886411D+02
0.4701701D+02	0.4518108D+02	0.4335769D+02	0.4154824D+02
0.3975410D+02	0.3797701D+02	0.3621844D+02	0.3448003D+02
0.3276347D+02	0.3107041D+02	0.2940283D+02	0.2776251D+02
0.2615132D+02	0.2457117D+02	0.2302416D+02	0.2151222D+02

A.3 PIXAN data files

0.2003747D+02	0.1860196D+02	0.1720778D+02	0.1652684D+02
0.1585703D+02	0.1519860D+02	0.1455182D+02	0.1391694D+02
0.1329422D+02	0.1268392D+02	0.1208628D+02	0.1150156D+02
0.1092999D+02	0.1037182D+02	0.9827284D+01	0.9296598D+01
0.8779986D+01	0.8277658D+01	0.7789814D+01	0.7316647D+01
0.6858337D+01	0.6415052D+01	0.5986947D+01	0.5574163D+01
0.5176824D+01	0.4795038D+01	0.4428896D+01	0.4078468D+01
0.3743803D+01	0.3424927D+01	0.3122293D+01	0.2834970D+01
0.2563358D+01	0.2307378D+01	0.2066924D+01	0.1841855D+01
0.1631997D+01	0.1437139D+01	0.1257035D+01	0.1091398D+01
0.9399023D+00	0.8021784D+00	0.6778153D+00	0.5663573D+00
0.4673040D+00	0.3801089D+00	0.3041804D+00	0.2388806D+00
0.1835282D+00	0.1374034D+00	0.9971946D-01	0.6968167D-01
0.4644909D-01	0.2915141D-01	0.1689596D-01	0.8777041D-02
0.3888540D-02	0.1342567D-02	0.3000004D-03	0.2735198D-04
0.2062635D-06			
40ZR			
89			
0.5716473D+02	0.5555470D+02	0.5394644D+02	0.5234070D+02
0.5073823D+02	0.4913970D+02	0.4754622D+02	0.4595851D+02
0.4437748D+02	0.4280407D+02	0.4123927D+02	0.3968410D+02
0.3813961D+02	0.3660680D+02	0.3508702D+02	0.3358134D+02
0.3209099D+02	0.3061722D+02	0.2916133D+02	0.2772458D+02
0.2630852D+02	0.2491447D+02	0.2354389D+02	0.2219820D+02
0.2087904D+02	0.1958785D+02	0.1832625D+02	0.1709581D+02
0.1589811D+02	0.1473477D+02	0.1360738D+02	0.1305767D+02
0.1251754D+02	0.1198720D+02	0.1146683D+02	0.1095663D+02
0.1045679D+02	0.9967500D+01	0.9488936D+01	0.9021281D+01
0.8564708D+01	0.8119389D+01	0.7685486D+01	0.7263159D+01
0.6852558D+01	0.6453826D+01	0.6067100D+01	0.5692506D+01
0.5330161D+01	0.4980171D+01	0.4642631D+01	0.4317624D+01
0.4005219D+01	0.3705472D+01	0.3418423D+01	0.3144097D+01
0.2882898D+01	0.2634014D+01	0.2397812D+01	0.2174241D+01
0.1963231D+01	0.1764687D+01	0.1578493D+01	0.1404504D+01
0.1242551D+01	0.1092438D+01	0.9539393D+00	0.8267998D+00
0.7107341D+00	0.6054255D+00	0.5105251D+00	0.4256512D+00
0.3503889D+00	0.2842902D+00	0.2268737D+00	0.1776251D+00
0.1360063D+00	0.1014191D+00	0.7326866D-01	0.5092127D-01
0.3371971D-01	0.2098724D-01	0.1203305D-01	0.6159407D-02
0.2671556D-02	0.8925858D-03	0.1885264D-03	0.1535100D-04
0.8545128D-07			
41NB			
89			
0.4707865D+02	0.4571024D+02	0.4434523D+02	0.4298414D+02
0.4162762D+02	0.4027638D+02	0.3893112D+02	0.3759260D+02
0.3626159D+02	0.3493889D+02	0.3362524D+02	0.3232169D+02
0.3102903D+02	0.2974819D+02	0.2848012D+02	0.2722578D+02
0.2598612D+02	0.2476232D+02	0.2355536D+02	0.2236635D+02
0.2119634D+02	0.2004657D+02	0.1891817D+02	0.1781228D+02
0.1673015D+02	0.1567298D+02	0.1464199D+02	0.1363842D+02
0.1266348D+02	0.1171843D+02	0.1080447D+02	0.1035953D+02
0.9922808D+01	0.9494458D+01	0.9074622D+01	0.8663442D+01
0.8261055D+01	0.7867599D+01	0.7483205D+01	0.7108001D+01
0.6742112D+01	0.6385656D+01	0.6038749D+01	0.5701498D+01
0.5374006D+01	0.5056369D+01	0.4748675D+01	0.4451005D+01
0.4163431D+01	0.3886016D+01	0.3618816D+01	0.3361872D+01
0.3115218D+01	0.2878875D+01	0.2653205D+01	0.2437491D+01
0.2232068D+01	0.2036903D+01	0.1851951D+01	0.1677145D+01
0.1512406D+01	0.1357636D+01	0.1212715D+01	0.1077507D+01
0.9518545D+00	0.8355792D+00	0.7284806D+00	0.6303357D+00
0.5408989D+00	0.4599005D+00	0.3870471D+00	0.3220208D+00
0.2644792D+00	0.2140554D+00	0.1703585D+00	0.1329740D+00
0.1014676D+00	0.7536598D-01	0.5419627D-01	0.3745876D-01
0.2463756D-01	0.1520382D-01	0.8619945D-02	0.4345138D-02
0.1843275D-02	0.5949511D-03	0.1184029D-03	0.8549903D-05
0.3436730D-07			

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42MO				
89				
0.3886078D+02	0.3769758D+02	0.3653861D+02	0.3538441D+02	
0.3423557D+02	0.3309267D+02	0.3195633D+02	0.3082710D+02	
0.2970581D+02	0.2859305D+02	0.2748952D+02	0.2639595D+02	
0.2531307D+02	0.2424165D+02	0.2318241D+02	0.2213630D+02	
0.2110406D+02	0.2008655D+02	0.1908459D+02	0.1809916D+02	
0.1713108D+02	0.1618131D+02	0.1525075D+02	0.1434036D+02	
0.1345107D+02	0.1258383D+02	0.1173960D+02	0.1091934D+02	
0.1012400D+02	0.9354499D+01	0.8611774D+01	0.8250734D+01	
0.7896723D+01	0.7549848D+01	0.7210217D+01	0.6877931D+01	
0.6553093D+01	0.6235798D+01	0.5926142D+01	0.5624215D+01	
0.5330104D+01	0.5043891D+01	0.4765654D+01	0.4495465D+01	
0.4233392D+01	0.3979497D+01	0.3733834D+01	0.3496453D+01	
0.3267395D+01	0.3046694D+01	0.2834377D+01	0.2630460D+01	
0.2435268D+01	0.2248164D+01	0.2069453D+01	0.1899113D+01	
0.1737113D+01	0.1583409D+01	0.1437943D+01	0.1300648D+01	
0.1171440D+01	0.1050222D+01	0.9368835D+00	0.8312972D+00	
0.7333212D+00	0.6427968D+00	0.5595488D+00	0.4833852D+00	
0.4140959D+00	0.3514537D+00	0.2952128D+00	0.2451095D+00	
0.2008621D+00	0.1621707D+00	0.1287179D+00	0.1001734D+00	
0.7617159D-01	0.5635289D-01	0.4033483D-01	0.2772186D-01	
0.1810732D-01	0.1107593D-01	0.6207105D-02	0.3079299D-02	
0.1276318D-02	0.3972842D-03	0.7432723D-04	0.4720214D-05	
0.1338622D-07				
43TC				
89				
0.3210319D+02	0.3111499D+02	0.3013156D+02	0.2915339D+02	
0.2818089D+02	0.2721471D+02	0.2625531D+02	0.2530322D+02	
0.2435899D+02	0.2342319D+02	0.2249641D+02	0.2157919D+02	
0.2067226D+02	0.1977621D+02	0.1889166D+02	0.1801929D+02	
0.1715974D+02	0.1631376D+02	0.1548201D+02	0.1466522D+02	
0.1386410D+02	0.1307938D+02	0.1231179D+02	0.1156208D+02	
0.1083098D+02	0.1011924D+02	0.9427600D+01	0.8756786D+01	
0.8107525D+01	0.7480524D+01	0.6876475D+01	0.6583267D+01	
0.6296044D+01	0.6014886D+01	0.5739870D+01	0.5471069D+01	
0.5208556D+01	0.4952399D+01	0.4702664D+01	0.4459414D+01	
0.4222707D+01	0.3992600D+01	0.3769143D+01	0.3552383D+01	
0.3342361D+01	0.3139116D+01	0.2942680D+01	0.2753078D+01	
0.2570331D+01	0.2394735D+01	0.2225733D+01	0.2063604D+01	
0.1908342D+01	0.1759933D+01	0.1618353D+01	0.1483573D+01	
0.1355552D+01	0.1234241D+01	0.1119582D+01	0.1011504D+01	
0.9099277D+00	0.8147628D+00	0.7259067D+00	0.6432455D+00	
0.5666529D+00	0.4959906D+00	0.4311072D+00	0.3718383D+00	
0.3180065D+00	0.2694209D+00	0.2258770D+00	0.1871568D+00	
0.1530289D+00	0.1232488D+00	0.9756250D-01	0.7569100D-01	
0.5735379D-01	0.4225882D-01	0.3010162D-01	0.2056853D-01	
0.1333828D-01	0.8083924D-02	0.4475428D-02	0.2183140D-02	
0.8829109D-03	0.2644357D-03	0.4626990D-04	0.2562590D-05	
0.4979626D-08				
44RU				
89				
0.2666268D+02	0.2582064D+02	0.2498371D+02	0.2415221D+02	
0.2332654D+02	0.2250715D+02	0.2169448D+02	0.2088897D+02	
0.2009104D+02	0.1930127D+02	0.1852011D+02	0.1774804D+02	
0.1698557D+02	0.1623320D+02	0.1549152D+02	0.1476105D+02	
0.1404231D+02	0.1333590D+02	0.1264237D+02	0.1196227D+02	
0.1129621D+02	0.1064474D+02	0.1000847D+02	0.9387962D+01	
0.8783806D+01	0.8196579D+01	0.7626852D+01	0.7075187D+01	
0.6542136D+01	0.6028232D+01	0.5533993D+01	0.5294402D+01	
0.5059910D+01	0.4830574D+01	0.4606450D+01	0.4387590D+01	
0.4174045D+01	0.3965863D+01	0.3763089D+01	0.3565767D+01	
0.3373936D+01	0.3187631D+01	0.3006885D+01	0.2831728D+01	
0.2662184D+01	0.2498274D+01	0.2340014D+01	0.2187669D+01	
0.2040738D+01	0.1899474D+01	0.1763872D+01	0.1633924D+01	
0.1509614D+01	0.1390920D+01	0.1277814D+01	0.1170260D+01	

A.3 PIXAN data files

0.1068217D+01	0.9716326D+00	0.8804509D+00	0.7946053D+00
0.7140217D+00	0.6386171D+00	0.5682997D+00	0.5029687D+00
0.4425135D+00	0.3868142D+00	0.3357411D+00	0.2891544D+00
0.2469042D+00	0.2088305D+00	0.1747631D+00	0.1445215D+00
0.1179152D+00	0.9474412D-01	0.7480113D-01	0.5785716D-01
0.4368949D-01	0.3206135D-01	0.2272845D-01	0.1543999D-01
0.9939849D-02	0.5968131D-02	0.3263213D-02	0.1564548D-02
0.6169164D-03	0.1775422D-03	0.2897652D-04	0.1390750D-05
0.1812340D-08			
45RH			
89			
0.2213927D+02	0.2142278D+02	0.2071135D+02	0.2000533D+02
0.1930507D+02	0.1861088D+02	0.1792323D+02	0.1724247D+02
0.1656896D+02	0.1590311D+02	0.1524529D+02	0.1459598D+02
0.1395556D+02	0.1332445D+02	0.1270311D+02	0.1209197D+02
0.1149147D+02	0.1090206D+02	0.1032419D+02	0.9758329D+01
0.9204925D+01	0.8664439D+01	0.8137330D+01	0.7624054D+01
0.7125063D+01	0.6640803D+01	0.6171711D+01	0.5718214D+01
0.5280728D+01	0.4859651D+01	0.4455364D+01	0.4259629D+01
0.4068225D+01	0.3881191D+01	0.3698566D+01	0.3520388D+01
0.3346692D+01	0.3177510D+01	0.3012872D+01	0.2852806D+01
0.2697338D+01	0.2546488D+01	0.2400278D+01	0.2258721D+01
0.2121833D+01	0.1989848D+01	0.1862316D+01	0.1739464D+01
0.1621292D+01	0.1507791D+01	0.1398951D+01	0.1294757D+01
0.1195187D+01	0.1100217D+01	0.1009813D+01	0.9239414D+00
0.8425580D+00	0.7656150D+00	0.6930577D+00	0.6248253D+00
0.5608503D+00	0.5010583D+00	0.4453682D+00	0.3936916D+00
0.3459329D+00	0.3019892D+00	0.2617498D+00	0.2250966D+00
0.1919037D+00	0.1620375D+00	0.1353567D+00	0.1117124D+00
0.9094831D-01	0.7290414D-01	0.5739878D-01	0.4425994D-01
0.3330298D-01	0.2433727D-01	0.1716676D-01	0.1159079D-01
0.7404980D-02	0.4402508D-02	0.2375703D-02	0.1118347D-02
0.4292518D-03	0.1183837D-03	0.1793257D-04	0.7376840D-06
0.6222573D-09			
46PD			
89			
0.1845354D+02	0.1784260D+02	0.1723657D+02	0.1663584D+02
0.1604065D+02	0.1545131D+02	0.1486813D+02	0.1429143D+02
0.1372150D+02	0.1315873D+02	0.1260342D+02	0.1205590D+02
0.11151654D+02	0.1098568D+02	0.1046366D+02	0.9950859D+01
0.9447620D+01	0.8954310D+01	0.8471292D+01	0.7998931D+01
0.7537590D+01	0.7087631D+01	0.6649413D+01	0.6223294D+01
0.5809621D+01	0.5408739D+01	0.5020982D+01	0.4646674D+01
0.4286125D+01	0.3939631D+01	0.3607471D+01	0.3446847D+01
0.3289902D+01	0.3136663D+01	0.2987159D+01	0.2841414D+01
0.2699451D+01	0.2561293D+01	0.2426958D+01	0.2296464D+01
0.2169826D+01	0.2047056D+01	0.1928369D+01	0.1813364D+01
0.1702246D+01	0.1595017D+01	0.1491677D+01	0.1392220D+01
0.1296639D+01	0.1204922D+01	0.1117055D+01	0.1033017D+01
0.9527872D+00	0.8763369D+00	0.8036354D+00	0.7346466D+00
0.6693301D+00	0.6076407D+00	0.5495283D+00	0.4949378D+00
0.4438086D+00	0.3960753D+00	0.3516666D+00	0.3105060D+00
0.2725110D+00	0.2375937D+00	0.2056601D+00	0.1766104D+00
0.1503392D+00	0.1267348D+00	0.1056798D+00	0.8705111D-01
0.7072069D-01	0.5655373D-01	0.4440616D-01	0.3413618D-01
0.2559388D-01	0.1862494D-01	0.1307109D-01	0.8770717D-02
0.5559642D-02	0.3272059D-02	0.1741860D-02	0.8045410D-03
0.3002687D-03	0.7920909D-04	0.1109565D-04	0.3879158D-06
0.2057894D-09			
47AG			
89			
0.1539198D+02	0.1487123D+02	0.1435522D+02	0.1384422D+02
0.1333846D+02	0.1283818D+02	0.1234369D+02	0.1185523D+02
0.1137305D+02	0.1089744D+02	0.1042868D+02	0.9967025D+01
0.9512774D+01	0.9066205D+01	0.8627605D+01	0.8197262D+01
0.7775466D+01	0.7362506D+01	0.6958671D+01	0.6564250D+01

A PIXAN PACKAGE

0.6179530D+01	0.5804795D+01	0.5440325D+01	0.5086395D+01
0.4743274D+01	0.4411225D+01	0.4090501D+01	0.3781343D+01
0.3483981D+01	0.3198633D+01	0.2925498D+01	0.2793568D+01
0.2664758D+01	0.2539087D+01	0.2416574D+01	0.2297235D+01
0.2181086D+01	0.2068138D+01	0.1958405D+01	0.1851895D+01
0.1748803D+01	0.1648761D+01	0.1551959D+01	0.1458396D+01
0.1368074D+01	0.1280987D+01	0.1197131D+01	0.1116497D+01
0.1039073D+01	0.9648453D+00	0.8937968D+00	0.8259072D+00
0.7611527D+00	0.6995066D+00	0.6409385D+00	0.5854145D+00
0.5328970D+00	0.4833446D+00	0.4367121D+00	0.3929503D+00
0.3520058D+00	0.3138211D+00	0.2783346D+00	0.2454800D+00
0.2151869D+00	0.1873804D+00	0.1619811D+00	0.1389051D+00
0.1180637D+00	0.9936427D-01	0.8270930D-01	0.6799701D-01
0.5512385D-01	0.4397242D-01	0.3443243D-01	0.2638562D-01
0.1971013D-01	0.1428083D-01	0.9969741D-02	0.6646440D-02
0.4178706D-02	0.2433279D-02	0.1276928D-02	0.5780732D-03
0.2094308D-03	0.5269497D-04	0.6790271D-05	0.1993680D-06
0.6393095D-10			
48CD			
89			
0.1285990D+02	0.1241580D+02	0.1197615D+02	0.1154123D+02
0.1111122D+02	0.1068631D+02	0.1026674D+02	0.9852713D+01
0.9444458D+01	0.9042195D+01	0.8646147D+01	0.8256543D+01
0.7873611D+01	0.7497582D+01	0.7128686D+01	0.6767155D+01
0.6413221D+01	0.6067114D+01	0.5729063D+01	0.5399297D+01
0.5078039D+01	0.4765512D+01	0.4461933D+01	0.4167514D+01
0.3882460D+01	0.3606969D+01	0.3341230D+01	0.3085425D+01
0.2839720D+01	0.2604271D+01	0.2379220D+01	0.2270634D+01
0.2164692D+01	0.2061408D+01	0.1960793D+01	0.1862858D+01
0.1767612D+01	0.1675228D+01	0.1585380D+01	0.1498237D+01
0.1413801D+01	0.1332074D+01	0.1253055D+01	0.1176742D+01
0.1103131D+01	0.1032214D+01	0.9639836D+00	0.8984286D+00
0.8355361D+00	0.7752906D+00	0.7176743D+00	0.6626668D+00
0.6102452D+00	0.5603837D+00	0.5130539D+00	0.4682245D+00
0.4258613D+00	0.3859270D+00	0.3483814D+00	0.3131809D+00
0.2802789D+00	0.2496254D+00	0.2211671D+00	0.1948473D+00
0.1706059D+00	0.1483793D+00	0.1281006D+00	0.1096991D+00
0.9310098D-01	0.7822871D-01	0.6500165D-01	0.5333836D-01
0.4314407D-01	0.3433226D-01	0.2680918D-01	0.2047819D-01
0.1524000D-01	0.1099288D-01	0.7632976D-02	0.5054684D-02
0.3151118D-02	0.1814739D-02	0.9382393D-03	0.4159314D-03
0.1460689D-03	0.3497010D-04	0.4126123D-05	0.1006512D-06
0.1879340D-10			
49IN			
89			
0.1076474D+02	0.1038573D+02	0.1001090D+02	0.9640423D+01
0.9274491D+01	0.8913268D+01	0.8556931D+01	0.8205661D+01
0.7859637D+01	0.7519044D+01	0.7184064D+01	0.6854882D+01
0.6531685D+01	0.6214657D+01	0.5903984D+01	0.5599852D+01
0.5302445D+01	0.5011946D+01	0.4728536D+01	0.4452393D+01
0.4183695D+01	0.3922611D+01	0.3669309D+01	0.3423951D+01
0.3186694D+01	0.2957684D+01	0.2737064D+01	0.2524965D+01
0.2321508D+01	0.2126802D+01	0.1940945D+01	0.1851361D+01
0.1764020D+01	0.1678928D+01	0.1596094D+01	0.1515674D+01
0.1437369D+01	0.1361333D+01	0.1287569D+01	0.1216078D+01
0.1146858D+01	0.1079090D+01	0.1015226D+01	0.9528052D+00
0.8926393D+00	0.8347201D+00	0.7790377D+00	0.7255802D+00
0.6743340D+00	0.6252835D+00	0.5784111D+00	0.5336971D+00
0.4911200D+00	0.4506557D+00	0.4122781D+00	0.3759589D+00
0.3416673D+00	0.3093702D+00	0.2790320D+00	0.2506146D+00
0.2240774D+00	0.1993772D+00	0.1764683D+00	0.1553021D+00
0.1358275D+00	0.1179908D+00	0.1017354D+00	0.8700204D-01
0.7372894D-01	0.6185167D-01	0.5130352D-01	0.4201514D-01
0.3391068D-01	0.2691802D-01	0.2096019D-01	0.1595804D-01
0.1183040D-01	0.8494280D-02	0.5865120D-02	0.3857064D-02
0.2383342D-02	0.1356788D-02	0.6905817D-03	0.2994580D-03

A.3 PIXAN data files

0.1017652D-03	0.2313687D-04	0.2483393D-05	0.4969006D-07
0.5167245D-11			
50SN			
89			
0.9030071D+01	0.8706285D+01	0.8386371D+01	0.8070471D+01
0.7758729D+01	0.7451289D+01	0.7148297D+01	0.6849902D+01
0.6556251D+01	0.6267493D+01	0.5983778D+01	0.5705256D+01
0.5432077D+01	0.5164389D+01	0.4902342D+01	0.4646084D+01
0.4395760D+01	0.4151516D+01	0.3913493D+01	0.3681832D+01
0.3456668D+01	0.3238134D+01	0.3026357D+01	0.2821461D+01
0.2623563D+01	0.2432773D+01	0.2249194D+01	0.2072921D+01
0.1904039D+01	0.1742624D+01	0.1588741D+01	0.1514640D+01
0.1442579D+01	0.1372286D+01	0.1303901D+01	0.1237427D+01
0.1172866D+01	0.1110218D+01	0.1049482D+01	0.9906583D+00
0.9337430D+00	0.8787323D+00	0.8256212D+00	0.7744031D+00
0.7250704D+00	0.6776139D+00	0.6320229D+00	0.5882856D+00
0.5463882D+00	0.5063156D+00	0.4680512D+00	0.4315765D+00
0.3968714D+00	0.3639141D+00	0.3326810D+00	0.3031466D+00
0.2752837D+00	0.2490629D+00	0.2244531D+00	0.2014211D+00
0.1799318D+00	0.1599481D+00	0.1414306D+00	0.1243381D+00
0.1086270D+00	0.9425201D-01	0.8116541D-01	0.6931753D-01
0.5865660D-01	0.4912893D-01	0.4068057D-01	0.3324853D-01
0.2677608D-01	0.2120158D-01	0.1646167D-01	0.1249131D-01
0.9223931D-02	0.6591595D-02	0.4525167D-02	0.2954549D-02
0.1808989D-02	0.1017497D-02	0.5094993D-03	0.2158895D-03
0.7087885D-04	0.1524686D-04	0.1482209D-05	0.2402384D-07
0.1330135D-11			
51SB			
89			
0.7591295D+01	0.7314393D+01	0.7041041D+01	0.6771358D+01
0.6505462D+01	0.6243473D+01	0.5985510D+01	0.5731695D+01
0.5482149D+01	0.5236994D+01	0.4996349D+01	0.4760337D+01
0.4529077D+01	0.4302690D+01	0.4081294D+01	0.3865007D+01
0.3653945D+01	0.3448220D+01	0.3247945D+01	0.3053228D+01
0.2864174D+01	0.2680884D+01	0.2503455D+01	0.2331981D+01
0.2166548D+01	0.2007236D+01	0.1854121D+01	0.1707269D+01
0.1566739D+01	0.1432581D+01	0.1304963D+01	0.1243504D+01
0.1183658D+01	0.1125427D+01	0.1068812D+01	0.1013813D+01
0.9604308D+00	0.9086628D+00	0.8585074D+00	0.8099615D+00
0.7630210D+00	0.7176808D+00	0.6739349D+00	0.6317760D+00
0.5911960D+00	0.5521855D+00	0.5147339D+00	0.4788293D+00
0.4444589D+00	0.4116084D+00	0.3802621D+00	0.3504032D+00
0.3220133D+00	0.2950728D+00	0.2695605D+00	0.2454538D+00
0.2227286D+00	0.2013594D+00	0.1813188D+00	0.1625783D+00
0.1451075D+00	0.1288744D+00	0.1138455D+00	0.9998559D-01
0.8725783D-01	0.7562379D-01	0.6504330D-01	0.5547468D-01
0.4687463D-01	0.3920036D-01	0.3240001D-01	0.2642853D-01
0.2123636D-01	0.1677254D-01	0.1298473D-01	0.9819326D-02
0.7221543D-02	0.5135542D-02	0.3504575D-02	0.2271160D-02
0.1377338D-02	0.7650254D-03	0.3765793D-03	0.1557429D-03
0.4930867D-04	0.1000456D-04	0.8756511D-06	0.1133660D-07
0.3175886D-12			
52TE			
89			
0.6395856D+01	0.6158769D+01	0.5924918D+01	0.5694401D+01
0.5467316D+01	0.5243760D+01	0.5023833D+01	0.4807633D+01
0.4595258D+01	0.4386808D+01	0.4182379D+01	0.3982069D+01
0.3785976D+01	0.3594195D+01	0.3406819D+01	0.3223943D+01
0.3045657D+01	0.2872050D+01	0.2703209D+01	0.2539218D+01
0.2380156D+01	0.2226102D+01	0.2077129D+01	0.1933304D+01
0.1794693D+01	0.1661353D+01	0.1533338D+01	0.1410692D+01
0.1293570D+01	0.1181775D+01	0.1075440D+01	0.1024325D+01
0.9745803D+00	0.9262057D+00	0.8792008D+00	0.8335647D+00
0.7892955D+00	0.7463908D+00	0.7048474D+00	0.6646612D+00
0.6258274D+00	0.5883404D+00	0.5521936D+00	0.5173797D+00
0.4838904D+00	0.4517165D+00	0.4208478D+00	0.3912730D+00

A PIXAN PACKAGE

0.3629802D+00	0.3359560D+00	0.3101862D+00	0.2856554D+00
0.2623471D+00	0.2402438D+00	0.2193268D+00	0.1995759D+00
0.1809703D+00	0.1634874D+00	0.1471037D+00	0.1317945D+00
0.1175335D+00	0.1042934D+00	0.9204560D-01	0.8076010D-01
0.7040567D-01	0.6094985D-01	0.5235872D-01	0.4459730D-01
0.3762966D-01	0.3141845D-01	0.2592218D-01	0.2110268D-01
0.1691878D-01	0.1332819D-01	0.1028756D-01	0.7752555D-02
0.5677934D-02	0.4017624D-02	0.2724847D-02	0.1752260D-02
0.1052167D-02	0.5768183D-03	0.2789156D-03	0.1124635D-03
0.3427681D-04	0.6540144D-05	0.5123988D-06	0.5225669D-08
0.7030172D-13			
53I			
89			
0.5398338D+01	0.5195157D+01	0.4994912D+01	0.4797682D+01
0.4603548D+01	0.4412590D+01	0.4224888D+01	0.4040523D+01
0.3859575D+01	0.3682123D+01	0.3508246D+01	0.3338024D+01
0.3171532D+01	0.3008846D+01	0.2850043D+01	0.2695194D+01
0.2544372D+01	0.2397644D+01	0.2255080D+01	0.2116741D+01
0.1982691D+01	0.1852987D+01	0.1727683D+01	0.1606829D+01
0.1490473D+01	0.1378655D+01	0.1271411D+01	0.1168878D+01
0.1070867D+01	0.9775001D+00	0.8887892D+00	0.8461808D+00
0.8047368D+00	0.7644564D+00	0.7253380D+00	0.6873796D+00
0.6505787D+00	0.6149320D+00	0.5804356D+00	0.5470851D+00
0.5148753D+00	0.4838003D+00	0.4538536D+00	0.4250279D+00
0.3973151D+00	0.3707065D+00	0.3451926D+00	0.3207628D+00
0.2974060D+00	0.2751102D+00	0.2538624D+00	0.2336489D+00
0.2144549D+00	0.1962648D+00	0.1790621D+00	0.1628294D+00
0.1475481D+00	0.1331988D+00	0.1197612D+00	0.1072138D+00
0.9553424D-01	0.8469905D-01	0.7468379D-01	0.6546300D-01
0.5701023D-01	0.4929793D-01	0.4229770D-01	0.3597989D-01
0.3031563D-01	0.2526954D-01	0.2081136D-01	0.1690769D-01
0.1352424D-01	0.1062582D-01	0.8176453D-02	0.6139349D-02
0.4477016D-02	0.3151311D-02	0.2123529D-02	0.1354527D-02
0.8048896D-03	0.4352042D-03	0.2065052D-03	0.8105785D-04
0.2372604D-04	0.4240150D-05	0.2950924D-06	0.2328068D-08
0.1406002D-13			
54XE			
89			
0.4550630D+01	0.4376792D+01	0.4205601D+01	0.4037124D+01
0.3871426D+01	0.3708572D+01	0.3548628D+01	0.3391659D+01
0.3237728D+01	0.3086901D+01	0.2939239D+01	0.2794806D+01
0.2653662D+01	0.2515867D+01	0.2381480D+01	0.2250558D+01
0.2123156D+01	0.1999327D+01	0.1879123D+01	0.1762591D+01
0.1649778D+01	0.1540727D+01	0.1435477D+01	0.1334064D+01
0.1236520D+01	0.1142970D+01	0.1053245D+01	0.9674568D+00
0.8856199D+00	0.8077417D+00	0.7338240D+00	0.6983491D+00
0.6638619D+00	0.6303609D+00	0.5978437D+00	0.5663078D+00
0.5357501D+00	0.5061670D+00	0.4775542D+00	0.4499070D+00
0.4232204D+00	0.3974883D+00	0.3727045D+00	0.3488619D+00
0.3259529D+00	0.3039694D+00	0.2829024D+00	0.2627425D+00
0.2434794D+00	0.2251023D+00	0.2075995D+00	0.1909589D+00
0.1751673D+00	0.1602111D+00	0.1460757D+00	0.1327459D+00
0.1202057D+00	0.1084383D+00	0.9742611D-01	0.8715070D-01
0.7759292D-01	0.6873279D-01	0.6054951D-01	0.5302153D-01
0.4612640D-01	0.3984098D-01	0.3414123D-01	0.2900330D-01
0.2440005D-01	0.2030492D-01	0.1669162D-01	0.1353234D-01
0.1079853D-01	0.8460971D-02	0.6489803D-02	0.4854542D-02
0.3524140D-02	0.2467030D-02	0.1651203D-02	0.1044301D-02
0.6137627D-03	0.3270660D-03	0.1521315D-03	0.5804053D-04
0.1627589D-04	0.2713132D-05	0.1663929D-06	0.9961992D-09
0.2509440D-14			
55CS			
89			
0.3880237D+01	0.3730141D+01	0.3582434D+01	0.3437169D+01
0.3294400D+01	0.3154181D+01	0.3016565D+01	0.2881606D+01
0.2749356D+01	0.2619866D+01	0.2493188D+01	0.2369370D+01

A.3 PIXAN data files

0.2248464D+01	0.2130515D+01	0.2015571D+01	0.1903676D+01
0.1794874D+01	0.1689205D+01	0.1586710D+01	0.1487426D+01
0.1391386D+01	0.1298623D+01	0.1209166D+01	0.1123041D+01
0.1040359D+01	0.9609602D+00	0.8849479D+00	0.8123326D+00
0.7431205D+00	0.6773130D+00	0.6149061D+00	0.5849752D+00
0.5558903D+00	0.5276495D+00	0.5002503D+00	0.4736896D+00
0.4479643D+00	0.4230705D+00	0.3990042D+00	0.3757605D+00
0.3533345D+00	0.3317206D+00	0.3109128D+00	0.2909044D+00
0.2716885D+00	0.2532575D+00	0.2356033D+00	0.2187172D+00
0.2025901D+00	0.1872122D+00	0.1725732D+00	0.1586621D+00
0.1454675D+00	0.1329773D+00	0.1211787D+00	0.1100584D+00
0.9960251D-01	0.8979637D-01	0.8062476D-01	0.7207182D-01
0.6412103D-01	0.5675521D-01	0.4995655D-01	0.4370662D-01
0.3798626D-01	0.3277581D-01	0.2805498D-01	0.2380320D-01
0.1999668D-01	0.1661453D-01	0.1363385D-01	0.1103116D-01
0.8782378D-02	0.6862901D-02	0.5247583D-02	0.3910778D-02
0.2826370D-02	0.1967816D-02	0.1308204D-02	0.8203294D-03
0.4768274D-03	0.2503892D-03	0.1141400D-03	0.4230678D-04
0.1135714D-04	0.1763269D-05	0.9498928D-07	0.4277852D-09
0.4311804D-15			
56BA			
89			
0.3283679D+01	0.3154970D+01	0.3028402D+01	0.2904018D+01
0.2781863D+01	0.2661979D+01	0.2544411D+01	0.2429199D+01
0.2316387D+01	0.2206015D+01	0.2098124D+01	0.1992754D+01
0.1889941D+01	0.1789725D+01	0.1692140D+01	0.1597222D+01
0.1505003D+01	0.1415514D+01	0.1328786D+01	0.1244844D+01
0.1163715D+01	0.1085422D+01	0.1010065D+01	0.9374991D+00
0.8678195D+00	0.8010373D+00	0.7371605D+00	0.6761934D+00
0.6181365D+00	0.5629859D+00	0.5107335D+00	0.4856903D+00
0.4613664D+00	0.4377596D+00	0.4148670D+00	0.3926856D+00
0.3712120D+00	0.3504425D+00	0.3303730D+00	0.3109990D+00
0.2923156D+00	0.2743176D+00	0.2569994D+00	0.2403548D+00
0.2243774D+00	0.2090604D+00	0.1943963D+00	0.1803775D+00
0.1669957D+00	0.1542423D+00	0.1421080D+00	0.1305833D+00
0.1196581D+00	0.1093218D+00	0.9956340D-01	0.9037126D-01
0.8173333D-01	0.7363703D-01	0.6606929D-01	0.5901649D-01
0.5246455D-01	0.4639878D-01	0.4080406D-01	0.3566471D-01
0.3096460D-01	0.2668698D-01	0.2281586D-01	0.1933062D-01
0.1621468D-01	0.1344933D-01	0.1101538D-01	0.8893165D-02
0.7062557D-02	0.5502996D-02	0.4193492D-02	0.3112645D-02
0.2238678D-02	0.1549459D-02	0.1022552D-02	0.6352841D-03
0.3648597D-03	0.1885591D-03	0.8408982D-04	0.3020412D-04
0.7731493D-05	0.1110646D-05	0.5190045D-07	0.1706465D-09
0.6138456D-16			
57LA			
89			
2.7960000D+00	2.6860000D+00	2.5760000D+00	2.4700000D+00
2.3640000D+00	2.2620000D+00	2.1600000D+00	2.0620000D+00
1.9650000D+00	1.8720000D+00	1.7780000D+00	1.6890000D+00
1.6000000D+00	1.5160000D+00	1.4310000D+00	1.3510000D+00
1.2710000D+00	1.1960000D+00	1.1210000D+00	1.0510000D+00
0.9807000D+00	0.9142000D+00	0.8501000D+00	0.7886000D+00
0.7295000D+00	0.6730000D+00	0.6189000D+00	0.5674000D+00
0.5183000D+00	0.4718000D+00	0.4277000D+00	0.4069000D+00
0.3861000D+00	0.3666000D+00	0.3470000D+00	0.3286000D+00
0.3102000D+00	0.2931000D+00	0.2759000D+00	0.2599000D+00
0.2439000D+00	0.2291000D+00	0.2143000D+00	0.2007000D+00
0.1870000D+00	0.1744000D+00	0.1618000D+00	0.1446000D+00
0.1389000D+00	0.1285000D+00	0.1181000D+00	0.1087000D+00
9.9340000D-02	9.0960000D-02	8.2570000D-02	7.5140000D-02
6.7710000D-02	6.1180000D-02	5.4660000D-02	4.9000000D-02
4.3340000D-02	3.8500000D-02	3.3650000D-02	2.9570000D-02
2.5490000D-02	2.2120000D-02	1.8740000D-02	1.6010000D-02
1.3280000D-02	1.1130000D-02	0.8990000D-02	0.7360000D-02
5.7360000D-03	4.5600000D-03	3.3840000D-03	2.5870000D-03

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1.7900000D-03	1.2980000D-03	8.0680000D-04	5.4420000D-04
2.8160000D-04	1.7200000D-04	6.2410000D-05	3.3840000D-05
5.2860000D-06	1.8070000D-07	2.8190000D-08	1.0000000D-11
1.0000000D-17			
58CE			
89			
2.3840000D-00	2.2900000D-00	2.1950000D-00	2.1040000D-00
2.0120000D-00	1.9250000D-00	1.8370000D-00	1.7530000D-00
1.6690000D-00	1.5890000D-00	1.5090000D-00	1.4320000D-00
1.3560000D-00	1.2840000D-00	1.2120000D-00	1.1430000D-00
1.0750000D-00	1.0110000D-00	9.4730000D-01	8.8760000D-01
8.2780000D-01	7.7130000D-01	7.1680000D-01	6.6460000D-01
6.1450000D-01	5.6650000D-01	5.2070000D-01	4.7700000D-01
4.3550000D-01	3.9730000D-01	3.5900000D-01	3.4140000D-01
3.2380000D-01	3.0730000D-01	2.9080000D-01	2.7540000D-01
2.5990000D-01	2.4540000D-01	2.3090000D-01	2.1740000D-01
2.0400000D-01	1.9150000D-01	1.7910000D-01	1.6760000D-01
1.5610000D-01	1.4560000D-01	1.3510000D-01	1.2540000D-01
1.1580000D-01	1.0710000D-01	9.8390000D-02	9.0540000D-02
8.2680000D-02	7.5660000D-02	6.8650000D-02	6.2440000D-02
5.6230000D-02	5.0780000D-02	4.5340000D-02	4.0620000D-02
3.5900000D-02	3.1860000D-02	2.7830000D-02	2.4440000D-02
2.1040000D-02	1.8230000D-02	1.5430000D-02	1.3160000D-02
1.0900000D-02	9.1260000D-03	7.3520000D-03	6.0100000D-03
4.6690000D-03	3.7030000D-03	2.7370000D-03	2.0140000D-03
1.4340000D-03	1.0350000D-03	6.3720000D-04	4.2730000D-04
2.1740000D-04	1.0950000D-04	4.6220000D-05	1.5900000D-05
3.5890000D-06	4.8460000D-07	1.4990000D-08	1.0000000D-11
1.0000000D-14			
59PR			
89			
2.0400000D-00	1.9580000D-00	1.8760000D-00	1.7970000D-00
1.7180000D-00	1.6420000D-00	1.5670000D-00	1.4950000D-00
1.4230000D-00	1.3540000D-00	1.2850000D-00	1.2190000D-00
1.1540000D-00	1.0920000D-00	1.0300000D-00	9.7160000D-01
9.1310000D-01	8.5840000D-01	8.0370000D-01	7.5260000D-01
7.0160000D-01	6.5330000D-01	6.0690000D-01	5.6230000D-01
5.1970000D-01	4.7880000D-01	4.3990000D-01	4.0280000D-01
3.6760000D-01	3.3420000D-01	3.0260000D-01	2.8770000D-01
2.7280000D-01	2.5880000D-01	2.4480000D-01	2.3170000D-01
2.1860000D-01	2.0640000D-01	1.9420000D-01	1.8280000D-01
1.7150000D-01	1.6100000D-01	1.5040000D-01	1.4070000D-01
1.3100000D-01	1.2220000D-01	1.1330000D-01	1.0520000D-01
9.7050000D-02	8.9710000D-02	8.2370000D-02	7.5760000D-02
6.9160000D-02	6.3260000D-02	5.7370000D-02	5.2160000D-02
4.6940000D-02	4.2370000D-02	3.7800000D-02	3.3840000D-02
2.9890000D-02	2.6510000D-02	2.3130000D-02	2.0290000D-02
1.7450000D-02	1.5110000D-02	1.2770000D-02	1.0880000D-02
8.9960000D-03	7.5200000D-03	6.0440000D-03	4.9320000D-03
3.8200000D-03	3.0220000D-03	2.2240000D-03	1.6300000D-03
1.1540000D-03	8.2960000D-04	5.0520000D-04	3.3670000D-04
1.6820000D-04	8.3300000D-05	3.4270000D-05	1.1390000D-05
2.4320000D-06	3.0280000D-07	7.8420000D-09	1.0000000D-11
1.0000000D-14			
60ND			
89			
1.7500000D-00	1.6800000D-00	1.6090000D-00	1.5400000D-00
1.4720000D-00	1.4070000D-00	1.3420000D-00	1.2800000D-00
1.2170000D-00	1.1580000D-00	1.0980000D-00	1.0420000D-00
9.8520000D-01	9.3190000D-01	8.7860000D-01	8.2850000D-01
7.7840000D-01	7.3140000D-01	6.8450000D-01	6.4070000D-01
5.9690000D-01	5.5560000D-01	5.1590000D-01	4.7780000D-01
4.4130000D-01	4.0650000D-01	3.7320000D-01	3.4160000D-01
3.1150000D-01	2.8310000D-01	2.5620000D-01	2.4360000D-01
2.3090000D-01	2.1900000D-01	2.0710000D-01	1.9600000D-01
1.8480000D-01	1.7440000D-01	1.6410000D-01	1.5440000D-01

A.3 PIXAN data files

1.4480000D-01	1.3580000D-01	1.2690000D-01	1.1870000D-01
1.1050000D-01	1.0300000D-01	9.5440000D-02	8.8580000D-02
8.1720000D-02	7.5510000D-02	6.9300000D-02	6.3720000D-02
5.8140000D-02	5.3160000D-02	4.8180000D-02	4.3780000D-02
3.9380000D-02	3.5520000D-02	3.1670000D-02	2.8340000D-02
2.5010000D-02	2.2160000D-02	1.9320000D-02	1.6940000D-02
1.4550000D-02	1.2580000D-02	1.0620000D-02	9.0410000D-03
7.4620000D-03	6.2280000D-03	4.9950000D-03	4.0680000D-03
3.1400000D-03	2.4780000D-03	1.8150000D-03	1.3240000D-03
9.3280000D-04	6.6740000D-04	4.0210000D-04	2.6640000D-04
1.3060000D-04	5.7640000D-05	2.5440000D-05	6.4630000D-06
1.6420000D-06	8.1370000D-08	4.0360000D-09	1.0000000D-12
1.0000000D-15			
-1ENER			
89			
0.6000000D+01	0.5900000D+01	0.5800000D+01	0.5700000D+01
0.5600000D+01	0.5500000D+01	0.5400000D+01	0.5300000D+01
0.5200000D+01	0.5100000D+01	0.5000000D+01	0.4900000D+01
0.4800000D+01	0.4700000D+01	0.4600000D+01	0.4500000D+01
0.4400000D+01	0.4300000D+01	0.4200000D+01	0.4100000D+01
0.4000000D+01	0.3900000D+01	0.3800000D+01	0.3700000D+01
0.3600000D+01	0.3500000D+01	0.3400000D+01	0.3300000D+01
0.3200000D+01	0.3100000D+01	0.3000000D+01	0.2950000D+01
0.2900000D+01	0.2850000D+01	0.2800000D+01	0.2750000D+01
0.2700000D+01	0.2650000D+01	0.2600000D+01	0.2550000D+01
0.2500000D+01	0.2450000D+01	0.2400000D+01	0.2350000D+01
0.2300000D+01	0.2250000D+01	0.2200000D+01	0.2150000D+01
0.2100000D+01	0.2050000D+01	0.2000000D+01	0.1950000D+01
0.1900000D+01	0.1850000D+01	0.1800000D+01	0.1750000D+01
0.1700000D+01	0.1650000D+01	0.1600000D+01	0.1550000D+01
0.1500000D+01	0.1450000D+01	0.1400000D+01	0.1350000D+01
0.1300000D+01	0.1250000D+01	0.1200000D+01	0.1150000D+01
0.1100000D+01	0.1050000D+01	0.1000000D+01	0.9500000D+00
0.9000000D+00	0.8500000D+00	0.8000000D+00	0.7500000D+00
0.7000000D+00	0.6500000D+00	0.6000000D+00	0.5500000D+00
0.5000000D+00	0.4500000D+00	0.4000000D+00	0.3500000D+00
0.3000000D+00	0.2500000D+00	0.2000000D+00	0.1500000D+00
0.1000000D+00			
42MOL			
89			
0.4248315D+05	0.4248164D+05	0.4247201D+05	0.4245380D+05
0.4242649D+05	0.4238954D+05	0.4234240D+05	0.4228444D+05
0.4221502D+05	0.4213348D+05	0.4203910D+05	0.4193107D+05
0.4180865D+05	0.4166973D+05	0.4151586D+05	0.4134478D+05
0.4115555D+05	0.4094704D+05	0.4071809D+05	0.4046747D+05
0.4019383D+05	0.3989587D+05	0.3957208D+05	0.3922089D+05
0.3884060D+05	0.3842956D+05	0.3798584D+05	0.3750749D+05
0.3699235D+05	0.3643836D+05	0.3584265D+05	0.3552883D+05
0.3520378D+05	0.3486709D+05	0.3451752D+05	0.3415684D+05
0.3378360D+05	0.3339744D+05	0.3299800D+05	0.3258484D+05
0.3215776D+05	0.3171631D+05	0.3126011D+05	0.3078880D+05
0.3030198D+05	0.2979920D+05	0.2928028D+05	0.2874476D+05
0.2819227D+05	0.2762248D+05	0.2703496D+05	0.2642959D+05
0.2580599D+05	0.2516380D+05	0.2450298D+05	0.2382321D+05
0.2312445D+05	0.2240663D+05	0.2166972D+05	0.2091382D+05
0.2013913D+05	0.1934596D+05	0.1853476D+05	0.1770614D+05
0.1686089D+05	0.1600004D+05	0.1512484D+05	0.1423684D+05
0.1333790D+05	0.1243025D+05	0.1151656D+05	0.1059993D+05
0.9684021D+04	0.8773017D+04	0.7871735D+04	0.6985727D+04
0.6120983D+04	0.5284357D+04	0.4483227D+04	0.3725459D+04
0.3019209D+04	0.2372683D+04	0.1793554D+04	0.1288494D+04
0.8632537D+03	0.5219656D+03	0.2673389D+03	0.1005990D+03
0.1850470D+02			
44RUL			
89			
0.3344334D+05	0.3339976D+05	0.3334880D+05	0.3329005D+05

A PIXAN PACKAGE

0.3322309D+05	0.3314752D+05	0.3306286D+05	0.3296770D+05
0.3286342D+05	0.3274850D+05	0.3262242D+05	0.3248458D+05
0.3233433D+05	0.3217101D+05	0.3199390D+05	0.3180232D+05
0.3159545D+05	0.3137249D+05	0.3113256D+05	0.3087471D+05
0.3059806D+05	0.3030157D+05	0.2998416D+05	0.2964467D+05
0.2928203D+05	0.2889494D+05	0.2848176D+05	0.2804189D+05
0.2757260D+05	0.2707434D+05	0.2654460D+05	0.2626743D+05
0.2598172D+05	0.2568743D+05	0.2538426D+05	0.2507202D+05
0.2475049D+05	0.2441947D+05	0.2407874D+05	0.2372803D+05
0.2336728D+05	0.2299621D+05	0.2261462D+05	0.2222231D+05
0.2181903D+05	0.2140474D+05	0.2097918D+05	0.2054221D+05
0.2009362D+05	0.1963341D+05	0.1916135D+05	0.1867746D+05
0.1818162D+05	0.1767384D+05	0.1715412D+05	0.1662252D+05
0.1607914D+05	0.1552417D+05	0.1495782D+05	0.1438042D+05
0.1379235D+05	0.1319412D+05	0.1258633D+05	0.1196970D+05
0.1134513D+05	0.1071364D+05	0.1007646D+05	0.9434981D+04
0.8790860D+04	0.8145970D+04	0.7502445D+04	0.6862734D+04
0.6229566D+04	0.5606028D+04	0.4995424D+04	0.4401486D+04
0.3828205D+04	0.3279830D+04	0.2760783D+04	0.2275564D+04
0.1828684D+04	0.1424262D+04	0.1065889D+04	0.7568004D+03
0.4994262D+03	0.2955213D+03	0.1462616D+03	0.5180278D+02
0.8391309D+01			
45RHL			
89			
0.2975664D+05	0.2969914D+05	0.2963467D+05	0.2956288D+05
0.2948256D+05	0.2939501D+05	0.2929894D+05	0.2919398D+05
0.2907965D+05	0.2895549D+05	0.2882098D+05	0.2867558D+05
0.2851880D+05	0.2835003D+05	0.2816866D+05	0.2797405D+05
0.2776549D+05	0.2754235D+05	0.2730384D+05	0.2704920D+05
0.2677759D+05	0.2648812D+05	0.2617999D+05	0.2585186D+05
0.2550346D+05	0.2513340D+05	0.2473979D+05	0.2432322D+05
0.2388167D+05	0.2341396D+05	0.2291880D+05	0.2266060D+05
0.2239509D+05	0.2212211D+05	0.2184150D+05	0.2155311D+05
0.2125671D+05	0.2095228D+05	0.2063959D+05	0.2031851D+05
0.1998886D+05	0.1965045D+05	0.1930328D+05	0.1894713D+05
0.1858189D+05	0.1820738D+05	0.1782362D+05	0.1743045D+05
0.1702777D+05	0.1661558D+05	0.1619384D+05	0.1576251D+05
0.1532163D+05	0.1487123D+05	0.1441141D+05	0.1394228D+05
0.1346403D+05	0.1297688D+05	0.1248113D+05	0.1197712D+05
0.1146530D+05	0.1094618D+05	0.1042040D+05	0.9888667D+04
0.9351845D+04	0.8810921D+04	0.8267027D+04	0.7721459D+04
0.7175703D+04	0.6631420D+04	0.6090505D+04	0.5555050D+04
0.5027412D+04	0.4510086D+04	0.4005890D+04	0.3517808D+04
0.3049059D+04	0.2602961D+04	0.2182891D+04	0.1792280D+04
0.1434424D+04	0.1112088D+04	0.8279834D+03	0.5842295D+03
0.3824185D+03	0.2236897D+03	0.1087551D+03	0.3735858D+02
0.5678593D+01			
46PDL			
89			
0.2649078D+05	0.2642282D+05	0.2634829D+05	0.2626692D+05
0.2617837D+05	0.2608229D+05	0.2597832D+05	0.2586608D+05
0.2574515D+05	0.2561517D+05	0.2547567D+05	0.2532620D+05
0.2516627D+05	0.2499535D+05	0.2481299D+05	0.2461859D+05
0.2441157D+05	0.2419134D+05	0.2395726D+05	0.2370861D+05
0.2344481D+05	0.2316478D+05	0.2286838D+05	0.2255447D+05
0.2222166D+05	0.2187044D+05	0.2149924D+05	0.2110714D+05
0.2069318D+05	0.2025652D+05	0.1979616D+05	0.1955679D+05
0.1931107D+05	0.1905901D+05	0.1880042D+05	0.1853519D+05
0.1826320D+05	0.1798434D+05	0.1769843D+05	0.1740550D+05
0.1710537D+05	0.1679796D+05	0.1648312D+05	0.1616087D+05
0.1583109D+05	0.1549368D+05	0.1514866D+05	0.1479594D+05
0.1443553D+05	0.1406742D+05	0.1369163D+05	0.1330819D+05
0.1291718D+05	0.1251869D+05	0.1211287D+05	0.1169988D+05
0.1127993D+05	0.1085331D+05	0.1042031D+05	0.9981337D+04
0.9536824D+04	0.9087301D+04	0.8633377D+04	0.8175754D+04
0.7715231D+04	0.7252733D+04	0.6789287D+04	0.6326071D+04

A.3 PIXAN data files

0.5864391D+04	0.5405719D+04	0.4951709D+04	0.4504061D+04
0.4064783D+04	0.3635979D+04	0.3219903D+04	0.2818985D+04
0.2435718D+04	0.2072674D+04	0.1732413D+04	0.1417516D+04
0.1130281D+04	0.8726989D+03	0.6466458D+03	0.4535464D+03
0.2944756D+03	0.1702146D+03	0.8121881D+02	0.2700465D+02
0.3833978D+01			
47AGL			
89			
0.2360988D+05	0.2353443D+05	0.2345288D+05	0.2336494D+05
0.2327032D+05	0.2316870D+05	0.2305981D+05	0.2294329D+05
0.2281879D+05	0.2268595D+05	0.2254439D+05	0.2239368D+05
0.2223346D+05	0.2206328D+05	0.2188267D+05	0.2169116D+05
0.2148821D+05	0.2127340D+05	0.2104587D+05	0.2080562D+05
0.2055177D+05	0.2028369D+05	0.2000024D+05	0.1970195D+05
0.1938753D+05	0.1905628D+05	0.1870744D+05	0.1834041D+05
0.1795440D+05	0.1754867D+05	0.1712243D+05	0.1690143D+05
0.1667505D+05	0.1644319D+05	0.1620577D+05	0.1596264D+05
0.1571383D+05	0.1545922D+05	0.1519872D+05	0.1493227D+05
0.1465975D+05	0.1438120D+05	0.1409651D+05	0.1380562D+05
0.1350854D+05	0.1320524D+05	0.1289570D+05	0.1257992D+05
0.1225793D+05	0.1192975D+05	0.1159544D+05	0.1125509D+05
0.1090880D+05	0.1055669D+05	0.1019895D+05	0.9835757D+04
0.9467362D+04	0.9094044D+04	0.8716135D+04	0.8334018D+04
0.7948138D+04	0.7559003D+04	0.7167194D+04	0.6773366D+04
0.6378267D+04	0.5982727D+04	0.5587677D+04	0.5194165D+04
0.4803330D+04	0.4416482D+04	0.4034931D+04	0.3660230D+04
0.3293988D+04	0.2937960D+04	0.2593978D+04	0.2263957D+04
0.1949862D+04	0.1653681D+04	0.1377411D+04	0.1122865D+04
0.8916462D+03	0.6853098D+03	0.5050838D+03	0.3519149D+03
0.2264982D+03	0.1293169D+03	0.6055812D+02	0.1950593D+02
0.2591645D+01			
48CDL			
89			
0.2099723D+05	0.2091650D+05	0.2083008D+05	0.2073777D+05
0.2063930D+05	0.2053439D+05	0.2042277D+05	0.2030415D+05
0.2017820D+05	0.2004465D+05	0.1990315D+05	0.1975336D+05
0.1959491D+05	0.1942745D+05	0.1925053D+05	0.1906359D+05
0.1886667D+05	0.1865908D+05	0.1844036D+05	0.1820946D+05
0.1796711D+05	0.1771218D+05	0.1744417D+05	0.1716253D+05
0.1686669D+05	0.1655619D+05	0.1623042D+05	0.1588882D+05
0.1553076D+05	0.1515579D+05	0.1476330D+05	0.1456032D+05
0.1435271D+05	0.1414050D+05	0.1392360D+05	0.1370193D+05
0.1347541D+05	0.1324407D+05	0.1300782D+05	0.1276662D+05
0.1252041D+05	0.1226921D+05	0.1201296D+05	0.1175168D+05
0.1148536D+05	0.1121399D+05	0.1093760D+05	0.1065623D+05
0.1036992D+05	0.1007874D+05	0.9782770D+04	0.9482121D+04
0.9176920D+04	0.8867323D+04	0.8553511D+04	0.8235701D+04
0.7914141D+04	0.7589120D+04	0.7260965D+04	0.6930056D+04
0.6596816D+04	0.6261725D+04	0.5925327D+04	0.5588221D+04
0.5251086D+04	0.4914662D+04	0.4579782D+04	0.4247340D+04
0.3918372D+04	0.3593883D+04	0.3275079D+04	0.2963194D+04
0.2659580D+04	0.2365626D+04	0.2082793D+04	0.1812574D+04
0.1556488D+04	0.1316048D+04	0.1092726D+04	0.8877089D+03
0.7022767D+03	0.5374556D+03	0.3940680D+03	0.2727460D+03
0.1739560D+03	0.9801422D+02	0.4496587D+02	0.1398184D+02
0.1725407D+01			
49INL			
89			
0.1868083D+05	0.1859682D+05	0.1850757D+05	0.1841288D+05
0.1831252D+05	0.1820623D+05	0.1809382D+05	0.1797501D+05
0.1784953D+05	0.1771712D+05	0.1757750D+05	0.1743032D+05
0.1727536D+05	0.1711206D+05	0.1694051D+05	0.1676014D+05
0.1657062D+05	0.1637105D+05	0.1616213D+05	0.1594291D+05
0.1571300D+05	0.1547200D+05	0.1521944D+05	0.1495498D+05
0.1467815D+05	0.1438851D+05	0.1408559D+05	0.1376903D+05
0.1343836D+05	0.1309311D+05	0.1273299D+05	0.1254721D+05

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0.1235756D+05	0.1216396D+05	0.1196645D+05	0.1176495D+05
0.1155943D+05	0.1134984D+05	0.1113621D+05	0.1091848D+05
0.1069667D+05	0.1047076D+05	0.1024075D+05	0.1000665D+05
0.9768478D+04	0.9526275D+04	0.9280078D+04	0.9029944D+04
0.8775942D+04	0.8518156D+04	0.8256690D+04	0.7991667D+04
0.7723227D+04	0.7451537D+04	0.7176790D+04	0.6899202D+04
0.6619024D+04	0.6336538D+04	0.6052060D+04	0.5765952D+04
0.5478607D+04	0.5190476D+04	0.4902046D+04	0.4613870D+04
0.4326539D+04	0.4040720D+04	0.3757149D+04	0.3476565D+04
0.3199826D+04	0.2927852D+04	0.2661594D+04	0.2402099D+04
0.2150433D+04	0.1907715D+04	0.1675092D+04	0.1453727D+04
0.1244788D+04	0.1049362D+04	0.8685471D+03	0.7031924D+03
0.5541999D+03	0.4222658D+03	0.3079454D+03	0.2116575D+03
0.1337142D+03	0.7431144D+02	0.3337465D+02	0.1000956D+02
0.1144725D+01			
50SNL			
89			
0.1662502D+05	0.1653932D+05	0.1644883D+05	0.1635334D+05
0.1625265D+05	0.1614657D+05	0.1603488D+05	0.1591736D+05
0.1579376D+05	0.1566390D+05	0.1552734D+05	0.1538418D+05
0.1523398D+05	0.1507647D+05	0.1491090D+05	0.1473795D+05
0.1455683D+05	0.1436724D+05	0.1416886D+05	0.1396135D+05
0.1374445D+05	0.1351780D+05	0.1328105D+05	0.1303389D+05
0.1277591D+05	0.1250687D+05	0.1222640D+05	0.1193412D+05
0.1162981D+05	0.1131312D+05	0.1098374D+05	0.1081425D+05
0.1064150D+05	0.1046548D+05	0.1028614D+05	0.1010350D+05
0.9917526D+04	0.9728222D+04	0.9535573D+04	0.9339580D+04
0.9140249D+04	0.8937593D+04	0.8731633D+04	0.8522397D+04
0.8309922D+04	0.8094256D+04	0.7875457D+04	0.7653594D+04
0.7428750D+04	0.7201024D+04	0.6970527D+04	0.6737390D+04
0.6501762D+04	0.6263811D+04	0.6023729D+04	0.5781731D+04
0.5538058D+04	0.5292980D+04	0.5046795D+04	0.4799837D+04
0.4552471D+04	0.4305105D+04	0.4058176D+04	0.3812175D+04
0.3567622D+04	0.3325123D+04	0.3085238D+04	0.2848659D+04
0.2616102D+04	0.2388319D+04	0.2166096D+04	0.1950281D+04
0.1741726D+04	0.1541319D+04	0.1349951D+04	0.1168527D+04
0.9978894D+03	0.8389008D+03	0.6922287D+03	0.5586049D+03
0.4386117D+03	0.3327241D+03	0.2413156D+03	0.1646724D+03
0.1030062D+03	0.5643125D+02	0.2479113D+02	0.7160410D+01
0.7562942D+00			
51SBL			
89			
0.1481460D+05	0.1472857D+05	0.1463812D+05	0.1454310D+05
0.1444334D+05	0.1433863D+05	0.1422885D+05	0.1411362D+05
0.1399308D+05	0.1386685D+05	0.1373473D+05	0.1359648D+05
0.1345156D+05	0.1330049D+05	0.1314264D+05	0.1297777D+05
0.1280564D+05	0.1262595D+05	0.1243854D+05	0.1224310D+05
0.1203938D+05	0.1182710D+05	0.1160598D+05	0.1137582D+05
0.1113631D+05	0.1088722D+05	0.1062824D+05	0.1035923D+05
0.1007988D+05	0.9790065D+04	0.9489551D+04	0.9335257D+04
0.9178233D+04	0.9018489D+04	0.8856007D+04	0.8690784D+04
0.8522816D+04	0.8352108D+04	0.8178668D+04	0.8002511D+04
0.7823658D+04	0.7642130D+04	0.7457964D+04	0.7271198D+04
0.7081882D+04	0.6890072D+04	0.6695839D+04	0.6499257D+04
0.6300420D+04	0.6099428D+04	0.5896402D+04	0.5691471D+04
0.5484785D+04	0.5276510D+04	0.5066831D+04	0.4855954D+04
0.4644107D+04	0.4431542D+04	0.4218534D+04	0.4005391D+04
0.3792439D+04	0.3580041D+04	0.3368594D+04	0.3158539D+04
0.2950299D+04	0.2744379D+04	0.2541314D+04	0.2341654D+04
0.2146004D+04	0.1954972D+04	0.1769221D+04	0.1589413D+04
0.1416235D+04	0.1250379D+04	0.1092555D+04	0.9433959D+03
0.8036356D+03	0.6737465D+03	0.5543394D+03	0.4458951D+03
0.3488163D+03	0.2634291D+03	0.1899881D+03	0.1286918D+03
0.7968557D+02	0.4302016D+02	0.1847912D+02	0.5136347D+01
0.5000062D+00			
52TEL			

A.3 PIXAN data files

89	0.1320870D+05	0.1312334D+05	0.1303393D+05	0.1294022D+05
	0.1284235D+05	0.1274001D+05	0.1263305D+05	0.1252131D+05
	0.1240461D+05	0.1228242D+05	0.1215533D+05	0.1202276D+05
	0.1188453D+05	0.1174046D+05	0.1159034D+05	0.1143396D+05
	0.1127117D+05	0.1110174D+05	0.1092547D+05	0.1074215D+05
	0.1055153D+05	0.1035348D+05	0.1014776D+05	0.9934166D+04
	0.9712474D+04	0.9482560D+04	0.9244215D+04	0.8997245D+04
	0.8741563D+04	0.8477000D+04	0.8203490D+04	0.8063361D+04
	0.7920974D+04	0.7776327D+04	0.7629421D+04	0.7480265D+04
	0.7328867D+04	0.7175241D+04	0.7019405D+04	0.6861382D+04
	0.6701201D+04	0.6538897D+04	0.6374511D+04	0.6208091D+04
	0.6039693D+04	0.5869380D+04	0.5697227D+04	0.5523315D+04
	0.5347738D+04	0.5170601D+04	0.4992020D+04	0.4812126D+04
	0.4631061D+04	0.4448988D+04	0.4266079D+04	0.4082530D+04
	0.3898549D+04	0.3714369D+04	0.3530244D+04	0.3346442D+04
	0.3163265D+04	0.2981026D+04	0.2800092D+04	0.2620798D+04
	0.2443548D+04	0.2268771D+04	0.2096901D+04	0.1928416D+04
	0.1763795D+04	0.1603556D+04	0.1448219D+04	0.1298313D+04
	0.1154393D+04	0.1016999D+04	0.8866292D+03	0.7638697D+03
	0.6490828D+03	0.5427648D+03	0.4453093D+03	0.3570520D+03
	0.2782743D+03	0.2091997D+03	0.1500067D+03	0.1008351D+03
	0.6178295D+02	0.3285223D+02	0.1378924D+02	0.3684187D+01
	0.3295893D+00			
53IL				
89				
	0.1177669D+05	0.1169283D+05	0.1160530D+05	0.1151398D+05
	0.1141875D+05	0.1131947D+05	0.1121567D+05	0.1110792D+05
	0.1099571D+05	0.1087890D+05	0.1075735D+05	0.1063091D+05
	0.1049939D+05	0.1036270D+05	0.1022065D+05	0.1007308D+05
	0.9919820D+04	0.9760686D+04	0.9595575D+04	0.9424291D+04
	0.9246675D+04	0.9062567D+04	0.8871783D+04	0.8674233D+04
	0.8469748D+04	0.8258170D+04	0.8039431D+04	0.7813385D+04
	0.7579978D+04	0.7339148D+04	0.7090856D+04	0.6963911D+04
	0.6835105D+04	0.6704445D+04	0.6571942D+04	0.6437608D+04
	0.6301459D+04	0.6163519D+04	0.6023812D+04	0.5882368D+04
	0.5739221D+04	0.5594413D+04	0.5447989D+04	0.5300003D+04
	0.5150515D+04	0.4999591D+04	0.4847306D+04	0.4693744D+04
	0.4538999D+04	0.4383173D+04	0.4226378D+04	0.4068742D+04
	0.3910399D+04	0.3751499D+04	0.3592209D+04	0.3432702D+04
	0.3273174D+04	0.3113832D+04	0.2954902D+04	0.2796631D+04
	0.2639290D+04	0.2483133D+04	0.2328465D+04	0.2175608D+04
	0.2024902D+04	0.1876692D+04	0.1731357D+04	0.1589274D+04
	0.1450852D+04	0.1316501D+04	0.1186633D+04	0.1061685D+04
	0.9420784D+03	0.8282036D+03	0.7205284D+03	0.6193293D+03
	0.5250085D+03	0.4378857D+03	0.3582386D+03	0.2863034D+03
	0.2222749D+03	0.1663085D+03	0.1185305D+03	0.7904074D+02
	0.4790040D+02	0.2507311D+02	0.1027465D+02	0.2634912D+01
	0.2158263D+00			
54XEL				
89				
	0.1049278D+05	0.1041105D+05	0.1032599D+05	0.1023719D+05
	0.1014518D+05	0.1004952D+05	0.9950102D+04	0.9846808D+04
	0.9739524D+04	0.9628102D+04	0.9512475D+04	0.9392491D+04
	0.9268025D+04	0.9138950D+04	0.9005138D+04	0.8866432D+04
	0.8722760D+04	0.8573965D+04	0.8419920D+04	0.8260474D+04
	0.8095558D+04	0.7925027D+04	0.7748771D+04	0.7566659D+04
	0.7378644D+04	0.7184602D+04	0.6984488D+04	0.6778246D+04
	0.6565837D+04	0.6347249D+04	0.6122503D+04	0.6007836D+04
	0.5891652D+04	0.5773964D+04	0.5654789D+04	0.5534145D+04
	0.5412055D+04	0.5288544D+04	0.5163643D+04	0.5037387D+04
	0.4909813D+04	0.4780968D+04	0.4650898D+04	0.4519660D+04
	0.4387315D+04	0.4253930D+04	0.4119579D+04	0.3984347D+04
	0.3848322D+04	0.3711604D+04	0.3574299D+04	0.3436525D+04
	0.3298413D+04	0.3160096D+04	0.3021728D+04	0.2883467D+04
	0.2745487D+04	0.2607979D+04	0.2471152D+04	0.2335192D+04

A PIXAN PACKAGE

0.2200344D+04	0.2066843D+04	0.1934950D+04	0.1804928D+04
0.1677062D+04	0.1551651D+04	0.1428991D+04	0.1309408D+04
0.1193221D+04	0.1080759D+04	0.9723506D+03	0.8683417D+03
0.7690288D+03	0.6747875D+03	0.5858254D+03	0.5024674D+03
0.4249704D+03	0.3535614D+03	0.2884369D+03	0.2297628D+03
0.1776744D+03	0.1322839D+03	0.9368399D+02	0.6194707D+02
0.37110902D+02	0.1910520D+02	0.7633798D+01	0.1874946D+01
0.1399252D+00			
55CSL			
89			
0.9353989D+04	0.9274891D+04	0.9192785D+04	0.9107583D+04
0.9019195D+04	0.8927529D+04	0.8832466D+04	0.8733959D+04
0.8631886D+04	0.8526147D+04	0.8416644D+04	0.8303274D+04
0.8185911D+04	0.8064503D+04	0.7938923D+04	0.7809069D+04
0.7674841D+04	0.7536115D+04	0.7392843D+04	0.7244908D+04
0.7092221D+04	0.6934676D+04	0.6772240D+04	0.6604807D+04
0.6432343D+04	0.6254798D+04	0.6072135D+04	0.5884339D+04
0.5691414D+04	0.5493390D+04	0.5290324D+04	0.5186926D+04
0.5082305D+04	0.4976477D+04	0.4869461D+04	0.4761280D+04
0.4651962D+04	0.4541534D+04	0.4430030D+04	0.4317487D+04
0.4203945D+04	0.4089450D+04	0.3974052D+04	0.3857807D+04
0.3740774D+04	0.3623021D+04	0.3504619D+04	0.3385648D+04
0.3266193D+04	0.3146347D+04	0.3026212D+04	0.2905895D+04
0.2785513D+04	0.2665195D+04	0.2545072D+04	0.2425293D+04
0.2306021D+04	0.2187397D+04	0.2069611D+04	0.1952843D+04
0.1837292D+04	0.1723168D+04	0.1610680D+04	0.1500063D+04
0.1391542D+04	0.1285370D+04	0.1181789D+04	0.1081065D+04
0.9834499D+03	0.8892058D+03	0.7986055D+03	0.7118797D+03
0.6293208D+03	0.5511165D+03	0.4774973D+03	0.4086812D+03
0.3448524D+03	0.2861734D+03	0.2327835D+03	0.1847983D+03
0.1423152D+03	0.1054143D+03	0.7416389D+02	0.4861497D+02
0.2877798D+02	0.1456943D+02	0.5674357D+01	0.1333866D+01
0.9047476D-01			
56BAL			
89			
0.8343342D+04	0.8267221D+04	0.8188389D+04	0.8106771D+04
0.8022271D+04	0.7934853D+04	0.7844418D+04	0.7750886D+04
0.7654177D+04	0.7554211D+04	0.7450883D+04	0.7344158D+04
0.7233931D+04	0.7120122D+04	0.7002650D+04	0.6881415D+04
0.6756385D+04	0.6627462D+04	0.6494576D+04	0.6357641D+04
0.6216634D+04	0.6071465D+04	0.5922116D+04	0.5768524D+04
0.5610676D+04	0.5448547D+04	0.5282137D+04	0.5111459D+04
0.4936550D+04	0.4757466D+04	0.4574294D+04	0.4481208D+04
0.4387145D+04	0.4292126D+04	0.4196173D+04	0.4099311D+04
0.4001567D+04	0.3902972D+04	0.3803562D+04	0.3703373D+04
0.3602447D+04	0.3500830D+04	0.3398570D+04	0.3295723D+04
0.3192345D+04	0.3088503D+04	0.2984263D+04	0.2879699D+04
0.2774894D+04	0.2669932D+04	0.2564905D+04	0.2459915D+04
0.2355065D+04	0.2250470D+04	0.2146265D+04	0.2042549D+04
0.1939473D+04	0.1837183D+04	0.1735826D+04	0.1635567D+04
0.1536568D+04	0.1439006D+04	0.1343068D+04	0.1248934D+04
0.1156808D+04	0.1066881D+04	0.9793641D+03	0.8944590D+03
0.8123841D+03	0.7333213D+03	0.6574855D+03	0.5851014D+03
0.5163141D+03	0.4513073D+03	0.3902578D+03	0.3333152D+03
0.2806129D+03	0.2322673D+03	0.1883763D+03	0.1490230D+03
0.1142767D+03	0.8419748D+02	0.5883539D+02	0.3822381D+02
0.2235410D+02	0.1112447D+02	0.4221065D+01	0.9486975D+00
0.5831287D-01			
57LAL			
89			
0.7465825D+04	0.7392859D+04	0.7317470D+04	0.7239577D+04
0.7159114D+04	0.7076019D+04	0.6990227D+04	0.6901651D+04
0.6810267D+04	0.6715990D+04	0.6618754D+04	0.6518493D+04
0.6415144D+04	0.6308622D+04	0.6198908D+04	0.6085920D+04
0.5969602D+04	0.5849883D+04	0.5726746D+04	0.5600117D+04
0.5469981D+04	0.5336285D+04	0.5199015D+04	0.5058150D+04

A.3 PIXAN data files

0.4913683D+04	0.4765620D+04	0.4613983D+04	0.4458807D+04
0.4300150D+04	0.4138089D+04	0.3972726D+04	0.3888847D+04
0.3804194D+04	0.3718788D+04	0.3632654D+04	0.3545817D+04
0.3458306D+04	0.3370154D+04	0.3281393D+04	0.3192061D+04
0.3102201D+04	0.3011853D+04	0.2921068D+04	0.2829897D+04
0.2738395D+04	0.2646621D+04	0.2554642D+04	0.2462525D+04
0.2370344D+04	0.2278180D+04	0.2186114D+04	0.2094237D+04
0.2002657D+04	0.1911451D+04	0.1820737D+04	0.1730631D+04
0.1641247D+04	0.1552713D+04	0.1465163D+04	0.1378728D+04
0.1293554D+04	0.1209792D+04	0.1127587D+04	0.1047106D+04
0.9685001D+03	0.8919414D+03	0.8175908D+03	0.7456239D+03
0.6761857D+03	0.6094483D+03	0.5455953D+03	0.4847396D+03
0.4270299D+03	0.3726113D+03	0.3216064D+03	0.2741258D+03
0.2302674D+03	0.1901145D+03	0.1537377D+03	0.1211979D+03
0.9254626D+02	0.6782753D+02	0.4707800D+02	0.3031675D+02
0.1751974D+02	0.8572854D+01	0.3170373D+01	0.6815046D+00
0.3795031D-01			
58CEL			
89			
0.6683395D+04	0.6613773D+04	0.6541957D+04	0.6467895D+04
0.6391533D+04	0.6312800D+04	0.6231682D+04	0.6148105D+04
0.6062018D+04	0.5973367D+04	0.5882083D+04	0.5788152D+04
0.5691505D+04	0.5592094D+04	0.5489856D+04	0.5384782D+04
0.5276814D+04	0.5165902D+04	0.5052038D+04	0.4935176D+04
0.4815304D+04	0.4692402D+04	0.4566463D+04	0.4437487D+04
0.4305486D+04	0.4170486D+04	0.4032523D+04	0.3891649D+04
0.3747939D+04	0.3601482D+04	0.3452394D+04	0.3376905D+04
0.3300814D+04	0.3224141D+04	0.3146912D+04	0.3069153D+04
0.2990892D+04	0.2912161D+04	0.2832992D+04	0.2753423D+04
0.2673492D+04	0.2593243D+04	0.2512719D+04	0.2431971D+04
0.2351050D+04	0.2270010D+04	0.2188912D+04	0.2107821D+04
0.2026801D+04	0.1945925D+04	0.1865281D+04	0.1784925D+04
0.1704955D+04	0.1625461D+04	0.1546533D+04	0.1468273D+04
0.1390784D+04	0.1314176D+04	0.1238555D+04	0.1164046D+04
0.1090761D+04	0.1018830D+04	0.9483814D+03	0.8795397D+03
0.8124429D+03	0.7472212D+03	0.6840161D+03	0.6229422D+03
0.5641390D+03	0.5077569D+03	0.4538831D+03	0.4026383D+03
0.3541414D+03	0.3084934D+03	0.2657853D+03	0.2260991D+03
0.1895056D+03	0.1560651D+03	0.1258305D+03	0.9884600D+02
0.7515125D+02	0.5478029D+02	0.3775920D+02	0.2409458D+02
0.1375478D+02	0.6614603D+01	0.2382149D+01	0.4889614D+00
0.2455716D-01			
59PRL			
89			
0.5987127D+04	0.5920904D+04	0.5852695D+04	0.5782495D+04
0.5710242D+04	0.5635893D+04	0.5559405D+04	0.5480736D+04
0.5399827D+04	0.5316671D+04	0.5231211D+04	0.5143408D+04
0.5053209D+04	0.4960610D+04	0.4865563D+04	0.4768025D+04
0.4667993D+04	0.4565425D+04	0.4460315D+04	0.4352643D+04
0.4242401D+04	0.4129588D+04	0.4014211D+04	0.3896286D+04
0.3775838D+04	0.3652905D+04	0.3527536D+04	0.3399798D+04
0.3269772D+04	0.3137557D+04	0.3003277D+04	0.2935406D+04
0.2867075D+04	0.2798305D+04	0.2729122D+04	0.2659551D+04
0.2589620D+04	0.2519359D+04	0.2448801D+04	0.2377979D+04
0.2306932D+04	0.2235699D+04	0.2164323D+04	0.2092849D+04
0.2021323D+04	0.1949801D+04	0.1878332D+04	0.1806976D+04
0.1735804D+04	0.1664860D+04	0.1594221D+04	0.1523958D+04
0.1454148D+04	0.1384867D+04	0.1316198D+04	0.1248228D+04
0.1181042D+04	0.1114735D+04	0.1049405D+04	0.9851449D+03
0.9220623D+03	0.8602540D+03	0.7998315D+03	0.7408959D+03
0.6835599D+03	0.6279360D+03	0.5741145D+03	0.5222084D+03
0.4723420D+03	0.4245815D+03	0.3790254D+03	0.3357712D+03
0.2949018D+03	0.2564923D+03	0.2206113D+03	0.1873187D+03
0.1566666D+03	0.1287011D+03	0.1034614D+03	0.8098313D+02
0.6129754D+02	0.4443237D+02	0.3040706D+02	0.1922053D+02
0.1083274D+02	0.5115648D+01	0.1791852D+01	0.3504025D+00

A PIXAN PACKAGE

0.1578929D-01				
60NDL				
89				
0.5388753D+04	0.5325873D+04	0.5261228D+04	0.5194783D+04	
0.5126503D+04	0.5056336D+04	0.4984280D+04	0.4910287D+04	
0.4834322D+04	0.4756353D+04	0.4676338D+04	0.4594273D+04	
0.4510119D+04	0.4423839D+04	0.4335431D+04	0.4244861D+04	
0.4152121D+04	0.4057195D+04	0.3960074D+04	0.3860755D+04	
0.3759241D+04	0.3655543D+04	0.3549677D+04	0.3441668D+04	
0.3331552D+04	0.3219376D+04	0.3105198D+04	0.2989090D+04	
0.2871138D+04	0.2751448D+04	0.2630144D+04	0.2568931D+04	
0.2507370D+04	0.2445482D+04	0.2383293D+04	0.2320827D+04	
0.2258110D+04	0.2195171D+04	0.2132040D+04	0.2068752D+04	
0.2005340D+04	0.1941841D+04	0.1878294D+04	0.1814743D+04	
0.1751230D+04	0.1687801D+04	0.1624515D+04	0.1561409D+04	
0.1498542D+04	0.1435973D+04	0.1373764D+04	0.1311976D+04	
0.1250675D+04	0.1189932D+04	0.1129814D+04	0.1070399D+04	
0.1011765D+04	0.9539857D+03	0.8971463D+03	0.8413326D+03	
0.7866243D+03	0.7331134D+03	0.6808825D+03	0.6300319D+03	
0.5806326D+03	0.5327787D+03	0.4865565D+03	0.4420701D+03	
0.3993647D+03	0.3585414D+03	0.3196622D+03	0.2828029D+03	
0.2480269D+03	0.2153912D+03	0.1849484D+03	0.1567431D+03	
0.1308149D+03	0.1071987D+03	0.8592476D+02	0.6702095D+02	
0.5051216D+02	0.3641935D+02	0.2475470D+02	0.1550977D+02	
0.8637713D+01	0.4010629D+01	0.1368671D+01	0.2555941D+00	
0.1036619D-01				
62SML				
89				
0.4346442D+04	0.4290295D+04	0.4232744D+04	0.4173766D+04	
0.4113339D+04	0.4051430D+04	0.3988044D+04	0.3923148D+04	
0.3856723D+04	0.3788746D+04	0.3719217D+04	0.3648110D+04	
0.3575422D+04	0.3501140D+04	0.3425257D+04	0.3347770D+04	
0.3268679D+04	0.3187987D+04	0.3105704D+04	0.3021842D+04	
0.2936420D+04	0.2849463D+04	0.2761002D+04	0.2671076D+04	
0.2579734D+04	0.2487031D+04	0.2393036D+04	0.2297827D+04	
0.2201496D+04	0.2104147D+04	0.2005903D+04	0.1956486D+04	
0.1906899D+04	0.1857160D+04	0.1807291D+04	0.1757316D+04	
0.1707255D+04	0.1657137D+04	0.1606986D+04	0.1556833D+04	
0.1506705D+04	0.1456634D+04	0.1406659D+04	0.1356803D+04	
0.1307107D+04	0.1257608D+04	0.1208347D+04	0.1159367D+04	
0.1110707D+04	0.1062414D+04	0.1014536D+04	0.9671174D+03	
0.9202100D+03	0.8738654D+03	0.8281380D+03	0.7830788D+03	
0.7387475D+03	0.6951958D+03	0.6524843D+03	0.6106734D+03	
0.5698234D+03	0.5299853D+03	0.4912226D+03	0.4535909D+03	
0.4171505D+03	0.3819727D+03	0.3480816D+03	0.3155503D+03	
0.2844174D+03	0.2547360D+03	0.2265498D+03	0.1998987D+03	
0.1748203D+03	0.1513468D+03	0.1295075D+03	0.1093288D+03	
0.9083370D+02	0.7404317D+02	0.5897693D+02	0.4565310D+02	
0.3408775D+02	0.2429251D+02	0.1626830D+02	0.9998454D+01	
0.5425556D+01	0.2428046D+01	0.7828760D+00	0.1322160D+00	
0.4260053D-02				
64GDL				
89				
0.3515369D+04	0.3465650D+04	0.3414823D+04	0.3362876D+04	
0.3309790D+04	0.3255567D+04	0.3200187D+04	0.3143648D+04	
0.3085937D+04	0.3027049D+04	0.2966978D+04	0.2905722D+04	
0.2843281D+04	0.2779655D+04	0.2714849D+04	0.2648870D+04	
0.2581729D+04	0.2513439D+04	0.2444019D+04	0.2373490D+04	
0.2301881D+04	0.2229223D+04	0.2155555D+04	0.2080923D+04	
0.2005379D+04	0.1928981D+04	0.1851800D+04	0.1773912D+04	
0.1695406D+04	0.1616380D+04	0.1536945D+04	0.1497112D+04	
0.1457224D+04	0.1417298D+04	0.1377353D+04	0.1337410D+04	
0.1297487D+04	0.1257610D+04	0.1217793D+04	0.1178065D+04	
0.1138448D+04	0.1098968D+04	0.1059652D+04	0.1020530D+04	
0.9816270D+03	0.9429741D+03	0.9046028D+03	0.8665465D+03	
0.8288350D+03	0.7915040D+03	0.7545902D+03	0.7181265D+03	

A.3 PIXAN data files

0.6821514D+03	0.6467024D+03	0.6118202D+03	0.5775398D+03
0.5439047D+03	0.5109557D+03	0.4787264D+03	0.4472602D+03
0.4165963D+03	0.3867747D+03	0.3578348D+03	0.3298277D+03
0.3027646D+03	0.2766984D+03	0.2516543D+03	0.2276693D+03
0.2047737D+03	0.1829955D+03	0.1623616D+03	0.1428952D+03
0.1246180D+03	0.1075491D+03	0.9170639D+02	0.7710566D+02
0.6376209D+02	0.5168945D+02	0.4090129D+02	0.3140993D+02
0.2322528D+02	0.1635133D+02	0.1078398D+02	0.6497122D+01
0.3432334D+01	0.1478578D+01	0.4493692D+00	0.6827335D-01
0.1721660D-02			
65TBL			
89			
0.3162577D+04	0.3115923D+04	0.3068284D+04	0.3019664D+04
0.2970043D+04	0.2919423D+04	0.2867792D+04	0.2815145D+04
0.2761478D+04	0.2706789D+04	0.2651077D+04	0.2594343D+04
0.2536591D+04	0.2477825D+04	0.2418053D+04	0.2357287D+04
0.2295540D+04	0.2232830D+04	0.2169177D+04	0.2104606D+04
0.2039148D+04	0.1972837D+04	0.1905713D+04	0.1837823D+04
0.1769217D+04	0.1699957D+04	0.1630109D+04	0.1559749D+04
0.1488960D+04	0.1417838D+04	0.1346484D+04	0.1310757D+04
0.1275017D+04	0.1239279D+04	0.1203561D+04	0.1167885D+04
0.1132260D+04	0.1096712D+04	0.1061258D+04	0.1025921D+04
0.9907229D+03	0.9556875D+03	0.9208359D+03	0.8861942D+03
0.8517877D+03	0.8176442D+03	0.7837877D+03	0.7502478D+03
0.7170529D+03	0.6842349D+03	0.6518203D+03	0.6198414D+03
0.5883321D+03	0.5573205D+03	0.5268410D+03	0.4969281D+03
0.4676157D+03	0.4389318D+03	0.4109115D+03	0.3835879D+03
0.3569938D+03	0.3311619D+03	0.3061353D+03	0.2819211D+03
0.2585646D+03	0.2360859D+03	0.2145160D+03	0.1938803D+03
0.1742022D+03	0.1555044D+03	0.1378065D+03	0.1211270D+03
0.1054822D+03	0.9088791D+02	0.7735771D+02	0.6490440D+02
0.5354055D+02	0.4327767D+02	0.3412708D+02	0.2609890D+02
0.1919966D+02	0.1343298D+02	0.8789252D+01	0.5241170D+01
0.2730773D+01	0.1153378D+01	0.3399220D+00	0.4886258D-01
0.1082625D-02			
66DYL			
89			
0.2802967D+04	0.2759582D+04	0.2715352D+04	0.2670267D+04
0.2624324D+04	0.2577517D+04	0.2529845D+04	0.2481306D+04
0.2431899D+04	0.2381627D+04	0.2330491D+04	0.2278498D+04
0.2225653D+04	0.2171965D+04	0.2117447D+04	0.2062112D+04
0.2005978D+04	0.1949064D+04	0.1891394D+04	0.1832997D+04
0.1773903D+04	0.1714148D+04	0.1653775D+04	0.1592830D+04
0.1531364D+04	0.1469436D+04	0.1407112D+04	0.1344463D+04
0.1281570D+04	0.1218520D+04	0.1155412D+04	0.1123869D+04
0.1092355D+04	0.1060878D+04	0.1029457D+04	0.9981074D+03
0.9668464D+03	0.9356915D+03	0.9046606D+03	0.8737733D+03
0.8430472D+03	0.8125032D+03	0.7821621D+03	0.7520465D+03
0.7221758D+03	0.6925736D+03	0.6632640D+03	0.6342719D+03
0.6056185D+03	0.5773306D+03	0.5494351D+03	0.5219544D+03
0.4949164D+03	0.4683492D+03	0.4422800D+03	0.4167309D+03
0.3917295D+03	0.3673057D+03	0.3434827D+03	0.3202884D+03
0.2977588D+03	0.2758982D+03	0.2547412D+03	0.2343152D+03
0.2146348D+03	0.1957255D+03	0.1776070D+03	0.1602989D+03
0.1438182D+03	0.1281808D+03	0.1134014D+03	0.9949359D+02
0.8646926D+02	0.7433933D+02	0.6311438D+02	0.5280375D+02
0.4341688D+02	0.3496240D+02	0.2744855D+02	0.2088202D+02
0.1526590D+02	0.1059959D+02	0.6869980D+01	0.4047417D+01
0.2075146D+01	0.8567719D+00	0.2437623D+00	0.3288250D-01
0.6271840D-03			
67HOL			
89			
0.2564372D+04	0.2523476D+04	0.2481821D+04	0.2439404D+04
0.2396222D+04	0.2352273D+04	0.2307556D+04	0.2262073D+04
0.2215825D+04	0.2168815D+04	0.2121049D+04	0.2072532D+04
0.2023274D+04	0.1973285D+04	0.1922578D+04	0.1871169D+04

A PIXAN PACKAGE

0.1819075D+04	0.1766318D+04	0.1712923D+04	0.1658917D+04
0.1604332D+04	0.1549204D+04	0.1493574D+04	0.1437486D+04
0.1380991D+04	0.1324145D+04	0.1267010D+04	0.1209655D+04
0.1152154D+04	0.1094591D+04	0.1037058D+04	0.1008330D+04
0.9796459D+03	0.9510205D+03	0.9224658D+03	0.8939978D+03
0.8656314D+03	0.8373833D+03	0.8092679D+03	0.7813031D+03
0.7535062D+03	0.7258953D+03	0.6984901D+03	0.6713072D+03
0.6443674D+03	0.6176906D+03	0.5912993D+03	0.5652112D+03
0.5394496D+03	0.5140376D+03	0.4889943D+03	0.4643438D+03
0.4401102D+03	0.4163170D+03	0.3929829D+03	0.3701314D+03
0.3477885D+03	0.3259740D+03	0.3047119D+03	0.2840340D+03
0.2639425D+03	0.2444682D+03	0.2256349D+03	0.2074550D+03
0.1899509D+03	0.1731403D+03	0.1570398D+03	0.1416654D+03
0.1270312D+03	0.1131509D+03	0.1000363D+03	0.8769922D+02
0.7614997D+02	0.6539815D+02	0.5545339D+02	0.4632442D+02
0.3802022D+02	0.3054908D+02	0.2391903D+02	0.1813565D+02
0.1320373D+02	0.9119830D+01	0.5871161D+01	0.3428291D+01
0.1736349D+01	0.7042570D+00	0.1947927D+00	0.2495483D-01
0.4217234D-03			
68ERL			
89			
0.2304143D+04	0.2265984D+04	0.2227164D+04	0.2187679D+04
0.2147530D+04	0.2106718D+04	0.2065243D+04	0.2023109D+04
0.1980320D+04	0.1936881D+04	0.1892799D+04	0.1848083D+04
0.1802743D+04	0.1756791D+04	0.1710243D+04	0.1663116D+04
0.1615428D+04	0.1567201D+04	0.1518462D+04	0.1469238D+04
0.1419562D+04	0.1369468D+04	0.1318997D+04	0.1268193D+04
0.1217103D+04	0.1165782D+04	0.1114287D+04	0.1062684D+04
0.1011042D+04	0.9594416D+03	0.9079577D+03	0.8822880D+03
0.8566820D+03	0.8311526D+03	0.8057119D+03	0.7803744D+03
0.7551516D+03	0.7300584D+03	0.7051094D+03	0.6803194D+03
0.6557048D+03	0.6312793D+03	0.6070600D+03	0.5830634D+03
0.5593081D+03	0.5358089D+03	0.5125845D+03	0.4896545D+03
0.4670342D+03	0.4447435D+03	0.4228028D+03	0.4012314D+03
0.3800425D+03	0.3592602D+03	0.3389020D+03	0.3189865D+03
0.2995325D+03	0.2805592D+03	0.2620936D+03	0.2441355D+03
0.2267116D+03	0.2098414D+03	0.1935349D+03	0.1778108D+03
0.1626836D+03	0.1481674D+03	0.1342754D+03	0.1210197D+03
0.1084116D+03	0.9646146D+02	0.8517938D+02	0.7457432D+02
0.6465473D+02	0.5542915D+02	0.4690543D+02	0.3909139D+02
0.3199492D+02	0.2562352D+02	0.1998392D+02	0.1508055D+02
0.1091641D+02	0.7486528D+01	0.4776686D+01	0.2757049D+01
0.1374746D+01	0.5452915D+00	0.1456514D+00	0.1751709D-01
0.2553634D-03			
69TML			
89			
0.2082416D+04	0.2046761D+04	0.2010526D+04	0.1973710D+04
0.1936315D+04	0.1898344D+04	0.1859799D+04	0.1820684D+04
0.1781006D+04	0.1740771D+04	0.1699988D+04	0.1658666D+04
0.1616818D+04	0.1574456D+04	0.1531597D+04	0.1488257D+04
0.1444457D+04	0.1400220D+04	0.1355570D+04	0.1310536D+04
0.1265149D+04	0.1219444D+04	0.1173459D+04	0.1127236D+04
0.1080821D+04	0.1034265D+04	0.9876220D+03	0.9409570D+03
0.8943267D+03	0.8478056D+03	0.8014678D+03	0.7783931D+03
0.7553956D+03	0.7324871D+03	0.7096771D+03	0.6869784D+03
0.6644030D+03	0.6419637D+03	0.6196741D+03	0.5975455D+03
0.57555925D+03	0.5538287D+03	0.5322700D+03	0.5109283D+03
0.4898197D+03	0.4689591D+03	0.4483634D+03	0.4280452D+03
0.4080217D+03	0.3883133D+03	0.3689266D+03	0.3498838D+03
0.3311986D+03	0.3128889D+03	0.2949693D+03	0.2774558D+03
0.2603645D+03	0.2437189D+03	0.2275175D+03	0.2117834D+03
0.1965334D+03	0.1817753D+03	0.1675252D+03	0.1537957D+03
0.1405983D+03	0.1279447D+03	0.1158450D+03	0.1043089D+03
0.9334531D+02	0.8296302D+02	0.7316968D+02	0.6397268D+02
0.5537895D+02	0.4739559D+02	0.4002906D+02	0.3328619D+02
0.2717330D+02	0.2169668D+02	0.1686090D+02	0.1267072D+02

A.3 PIXAN data files

0.9125469D+01	0.6219347D+01	0.3937181D+01	0.2249502D+01
0.1106301D+01	0.4301378D+00	0.1112942D+00	0.1261872D-01
0.1596614D-03			
70YBL			
89			
0.1878645D+04	0.1845402D+04	0.1811654D+04	0.1777402D+04
0.1742649D+04	0.1707398D+04	0.1671654D+04	0.1635423D+04
0.1598712D+04	0.1561528D+04	0.1523881D+04	0.1485782D+04
0.1447244D+04	0.1408280D+04	0.1368907D+04	0.1329143D+04
0.1289007D+04	0.1248524D+04	0.1207717D+04	0.1166614D+04
0.1125246D+04	0.1083646D+04	0.1041850D+04	0.9998987D+03
0.9578356D+03	0.9157079D+03	0.8735705D+03	0.8314717D+03
0.7894752D+03	0.7476437D+03	0.7060473D+03	0.6853607D+03
0.6647598D+03	0.6442555D+03	0.6238578D+03	0.6035774D+03
0.5834260D+03	0.5634127D+03	0.5435499D+03	0.5238488D+03
0.5043232D+03	0.4849826D+03	0.4658404D+03	0.4469094D+03
0.4282036D+03	0.4097334D+03	0.3915133D+03	0.3735608D+03
0.3558809D+03	0.3384908D+03	0.3214058D+03	0.3046377D+03
0.2882000D+03	0.2721059D+03	0.2563692D+03	0.2410030D+03
0.2260279D+03	0.2114409D+03	0.1972622D+03	0.1835062D+03
0.1701789D+03	0.1572940D+03	0.1448623D+03	0.1328934D+03
0.1213971D+03	0.1103822D+03	0.9985698D+02	0.8982910D+02
0.8030573D+02	0.7129399D+02	0.6280012D+02	0.5483014D+02
0.4739027D+02	0.4048610D+02	0.3412364D+02	0.2830847D+02
0.2304628D+02	0.1834219D+02	0.1419981D+02	0.1062248D+02
0.7608307D+01	0.5150357D+01	0.3232819D+01	0.1826791D+01
0.8850753D+00	0.3367714D+00	0.8419852D-01	0.8961668D-02
0.9752457D-04			
71LUL			
89			
0.1695962D+04	0.1664996D+04	0.1633591D+04	0.1601751D+04
0.1569478D+04	0.1536778D+04	0.1503657D+04	0.1470120D+04
0.1436177D+04	0.1401835D+04	0.1367104D+04	0.1331997D+04
0.1296527D+04	0.1260707D+04	0.1224555D+04	0.1188089D+04
0.1151328D+04	0.1114295D+04	0.1077014D+04	0.1039512D+04
0.1001817D+04	0.9639630D+03	0.9259840D+03	0.8879170D+03
0.8498038D+03	0.8116902D+03	0.7736185D+03	0.7356429D+03
0.6978168D+03	0.6601997D+03	0.6228541D+03	0.6043030D+03
0.5858447D+03	0.5674880D+03	0.5492429D+03	0.5311170D+03
0.5131206D+03	0.4952632D+03	0.4775566D+03	0.4600084D+03
0.4426302D+03	0.4254324D+03	0.4084271D+03	0.3916227D+03
0.3750314D+03	0.3586672D+03	0.3425370D+03	0.3266522D+03
0.3110270D+03	0.2956705D+03	0.2805956D+03	0.2658127D+03
0.2513331D+03	0.2371683D+03	0.2233292D+03	0.2098337D+03
0.1966785D+03	0.1838807D+03	0.1714527D+03	0.1593991D+03
0.1477318D+03	0.1364598D+03	0.1255913D+03	0.1151346D+03
0.1050972D+03	0.9548614D+02	0.8630812D+02	0.7756922D+02
0.6927572D+02	0.6143302D+02	0.5404639D+02	0.4712130D+02
0.4066273D+02	0.3467571D+02	0.2916546D+02	0.2413703D+02
0.1959523D+02	0.1554381D+02	0.1198712D+02	0.8925691D+01
0.6357199D+01	0.4273822D+01	0.2659426D+01	0.1485925D+01
0.7089869D+00	0.2638556D+00	0.6368039D-01	0.6349890D-02
0.5915015D-04			
72HFL			
89			
0.1525131D+04	0.1496383D+04	0.1467258D+04	0.1437760D+04
0.1407894D+04	0.1377666D+04	0.1347081D+04	0.1316148D+04
0.1284874D+04	0.1253269D+04	0.1221345D+04	0.1189112D+04
0.1156584D+04	0.1123777D+04	0.1090706D+04	0.1057389D+04
0.1023846D+04	0.9900982D+03	0.9561700D+03	0.9220862D+03
0.8878757D+03	0.8535677D+03	0.8191953D+03	0.7847968D+03
0.7504039D+03	0.7160603D+03	0.6818098D+03	0.6476987D+03
0.6137767D+03	0.5800971D+03	0.5467145D+03	0.5301531D+03
0.5136893D+03	0.4973292D+03	0.4810813D+03	0.4649546D+03
0.4489571D+03	0.4330983D+03	0.4173849D+03	0.4018268D+03
0.3864330D+03	0.3712136D+03	0.3561758D+03	0.3413324D+03

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0.3266889D+03	0.3122551D+03	0.2980419D+03	0.2840596D+03
0.2703158D+03	0.2568218D+03	0.2435859D+03	0.2306177D+03
0.2179266D+03	0.2055287D+03	0.1934196D+03	0.1816149D+03
0.1701230D+03	0.1589545D+03	0.1481127D+03	0.1376079D+03
0.1274475D+03	0.1176384D+03	0.1081876D+03	0.9910144D+02
0.9038574D+02	0.8204623D+02	0.7408810D+02	0.6651666D+02
0.5933654D+02	0.5255222D+02	0.4616841D+02	0.4018935D+02
0.3461933D+02	0.2946289D+02	0.2472425D+02	0.2040776D+02
0.1651740D+02	0.1305606D+02	0.1002688D+02	0.7429379D+01
0.5260206D+01	0.3510774D+01	0.2164831D+01	0.1195401D+01
0.5613158D+00	0.2041086D+00	0.4746814D-01	0.4419768D-02
0.3488492D-04			
73TAL			
89			
0.1372784D+04	0.1346114D+04	0.1319122D+04	0.1291813D+04
0.1264191D+04	0.1236265D+04	0.1208039D+04	0.1179522D+04
0.1150724D+04	0.1121653D+04	0.1092322D+04	0.1062741D+04
0.1032925D+04	0.1002888D+04	0.9726459D+03	0.9422164D+03
0.9116191D+03	0.8808740D+03	0.8500042D+03	0.8190343D+03
0.7879900D+03	0.7569024D+03	0.7257975D+03	0.6947096D+03
0.6636744D+03	0.6327284D+03	0.6019122D+03	0.5712683D+03
0.5408404D+03	0.5106764D+03	0.4808268D+03	0.4660354D+03
0.4513421D+03	0.4367541D+03	0.4222783D+03	0.4079228D+03
0.3936929D+03	0.3795972D+03	0.3656431D+03	0.3518393D+03
0.3381916D+03	0.3247110D+03	0.3114018D+03	0.2982722D+03
0.2853315D+03	0.2725885D+03	0.2600494D+03	0.2477237D+03
0.2356185D+03	0.2237418D+03	0.2121016D+03	0.2007060D+03
0.1895685D+03	0.1786848D+03	0.1680681D+03	0.1577254D+03
0.1476658D+03	0.1378919D+03	0.1284124D+03	0.1192332D+03
0.1103607D+03	0.1018004D+03	0.9355756D+02	0.8563734D+02
0.7804457D+02	0.7078367D+02	0.6385923D+02	0.5727525D+02
0.5103572D+02	0.4514441D+02	0.3960538D+02	0.3442224D+02
0.2959899D+02	0.2513937D+02	0.2104728D+02	0.1732641D+02
0.1397964D+02	0.1101060D+02	0.8420100D+01	0.6207369D+01
0.4368286D+01	0.2893777D+01	0.1767700D+01	0.9642828D+00
0.4453501D+00	0.1580917D+00	0.3537947D-01	0.3067449D-02
0.2042142D-04			
74WL			
89			
0.1237594D+04	0.1212857D+04	0.1187845D+04	0.1162564D+04
0.1137021D+04	0.1111221D+04	0.1085173D+04	0.1058883D+04
0.1032362D+04	0.1005619D+04	0.9786649D+03	0.9515125D+03
0.9241748D+03	0.8966658D+03	0.8690016D+03	0.8411988D+03
0.8132757D+03	0.7852528D+03	0.7571507D+03	0.7289927D+03
0.7008061D+03	0.6726122D+03	0.6444417D+03	0.6163252D+03
0.5882942D+03	0.5603832D+03	0.5326289D+03	0.5050682D+03
0.4777421D+03	0.4506934D+03	0.4239652D+03	0.4107360D+03
0.3976054D+03	0.3845778D+03	0.3716603D+03	0.3588590D+03
0.3461804D+03	0.3336318D+03	0.3212180D+03	0.3089484D+03
0.2968258D+03	0.2848595D+03	0.2730549D+03	0.2614202D+03
0.2499606D+03	0.2386843D+03	0.2275970D+03	0.2167062D+03
0.2060180D+03	0.1955394D+03	0.1852826D+03	0.1752428D+03
0.1654319D+03	0.1558561D+03	0.1465212D+03	0.1374351D+03
0.1285997D+03	0.1200223D+03	0.1117080D+03	0.1036622D+03
0.9588951D+02	0.8839445D+02	0.8118142D+02	0.7425451D+02
0.6761752D+02	0.6127445D+02	0.5522874D+02	0.4948385D+02
0.4404308D+02	0.3890996D+02	0.3408765D+02	0.2957965D+02
0.2538924D+02	0.2151989D+02	0.1797494D+02	0.1475756D+02
0.1187009D+02	0.9315362D+01	0.7093547D+01	0.5203150D+01
0.3639457D+01	0.2393102D+01	0.1448251D+01	0.7804719D+00
0.3545271D+00	0.1228434D+00	0.2644328D-01	0.2132418D-02
0.1193378D-04			
760SL			
89			
0.1006138D+04	0.9849185D+03	0.9635054D+03	0.9419040D+03
0.9201204D+03	0.8981619D+03	0.8760360D+03	0.8537512D+03

A.3 PIXAN data files

0.8313161D+03	0.8087411D+03	0.7860365D+03	0.7632141D+03
0.7402857D+03	0.7172654D+03	0.6941674D+03	0.6710068D+03
0.6478022D+03	0.6245677D+03	0.6013233D+03	0.5780896D+03
0.5548880D+03	0.5317405D+03	0.5086714D+03	0.4857059D+03
0.4628712D+03	0.4401943D+03	0.4177050D+03	0.3954349D+03
0.3734146D+03	0.3516792D+03	0.3302616D+03	0.3196834D+03
0.3091984D+03	0.2988118D+03	0.2885269D+03	0.2783511D+03
0.2682853D+03	0.2583369D+03	0.2485094D+03	0.2388084D+03
0.2292394D+03	0.2198058D+03	0.2105137D+03	0.2013673D+03
0.1923714D+03	0.1835311D+03	0.1748512D+03	0.1663411D+03
0.1579958D+03	0.1498249D+03	0.1418326D+03	0.1340234D+03
0.1264032D+03	0.1189728D+03	0.1117379D+03	0.1047024D+03
0.9786987D+02	0.9124426D+02	0.8482882D+02	0.7862691D+02
0.7264164D+02	0.6687605D+02	0.6133291D+02	0.5601525D+02
0.5092562D+02	0.4606663D+02	0.4144075D+02	0.3705072D+02
0.3289897D+02	0.2898801D+02	0.2532056D+02	0.2189915D+02
0.1872652D+02	0.1580528D+02	0.1313752D+02	0.1072628D+02
0.8572821D+01	0.6677956D+01	0.5041130D+01	0.3659756D+01
0.2528341D+01	0.1637397D+01	0.9721209D+00	0.5109617D+00
0.2243035D+00	0.7392590D-01	0.1467759D-01	0.1017353D-02
0.3960142D-05			
77IRL			
89			
0.9062255D+03	0.8866162D+03	0.8668464D+03	0.8469217D+03
0.8268485D+03	0.8066340D+03	0.7862856D+03	0.7658117D+03
0.7452210D+03	0.7245233D+03	0.7037284D+03	0.6828480D+03
0.6618938D+03	0.6408784D+03	0.6198171D+03	0.5987211D+03
0.5776078D+03	0.5564932D+03	0.5353949D+03	0.5143318D+03
0.4933228D+03	0.4723891D+03	0.4515528D+03	0.4308359D+03
0.4102628D+03	0.3898596D+03	0.3696510D+03	0.3496655D+03
0.3299319D+03	0.3104783D+03	0.2913356D+03	0.2818913D+03
0.2725375D+03	0.2632756D+03	0.2541112D+03	0.2450489D+03
0.2360918D+03	0.2272445D+03	0.2185118D+03	0.2098964D+03
0.2014038D+03	0.1930369D+03	0.1848008D+03	0.1766990D+03
0.1687357D+03	0.1609151D+03	0.1532454D+03	0.1457219D+03
0.1383526D+03	0.1311413D+03	0.1240918D+03	0.1172091D+03
0.1104936D+03	0.1039502D+03	0.9758221D+02	0.9139298D+02
0.8538537D+02	0.7956237D+02	0.7392674D+02	0.6848120D+02
0.6322820D+02	0.5817047D+02	0.5331026D+02	0.4864992D+02
0.4419170D+02	0.3993775D+02	0.3589046D+02	0.3205196D+02
0.2842443D+02	0.2501029D+02	0.2181175D+02	0.1883123D+02
0.1607106D+02	0.1353353D+02	0.1122043D+02	0.9134258D+01
0.7275871D+01	0.5645595D+01	0.4242401D+01	0.3063303D+01
0.2102588D+01	0.1350875D+01	0.7940101D+00	0.4119133D+00
0.1776030D+00	0.5700994D-01	0.1084603D-01	0.6938679D-03
0.2230042D-05			
78PTL			
89			
0.8170587D+03	0.7989434D+03	0.7806962D+03	0.7623234D+03
0.7438311D+03	0.7252264D+03	0.7065165D+03	0.6877096D+03
0.6688142D+03	0.6498397D+03	0.6307958D+03	0.6116933D+03
0.5925449D+03	0.5733593D+03	0.5541514D+03	0.5349342D+03
0.5157224D+03	0.4965310D+03	0.4773769D+03	0.4582762D+03
0.4392472D+03	0.4203091D+03	0.4014809D+03	0.3827839D+03
0.3642400D+03	0.3458707D+03	0.3277001D+03	0.3097532D+03
0.2920536D+03	0.2746279D+03	0.2575048D+03	0.2490632D+03
0.2407070D+03	0.2324399D+03	0.2242646D+03	0.2161850D+03
0.2082052D+03	0.2003275D+03	0.1925560D+03	0.1848948D+03
0.1773465D+03	0.1699149D+03	0.1626034D+03	0.1554155D+03
0.1483586D+03	0.1414282D+03	0.1346314D+03	0.1279715D+03
0.1214516D+03	0.1150748D+03	0.1088456D+03	0.1027640D+03
0.9683441D+02	0.9105946D+02	0.8544207D+02	0.7998465D+02
0.7468976D+02	0.6955973D+02	0.6459689D+02	0.5980333D+02
0.5518144D+02	0.5073315D+02	0.4646049D+02	0.4236542D+02
0.3844983D+02	0.3471581D+02	0.3116523D+02	0.2779999D+02
0.2462224D+02	0.2163392D+02	0.1883717D+02	0.1623409D+02

A PIXAN PACKAGE

0.1382674D+02	0.1161677D+02	0.9606676D+01	0.7797493D+01
0.6190048D+01	0.4784251D+01	0.3578683D+01	0.2570062D+01
0.1752560D+01	0.1117001D+01	0.6499401D+00	0.3327399D+00
0.1408775D+00	0.4402438D-01	0.8018653D-02	0.4726925D-03
0.1249729D-05			
79AUL			
89			
0.7376585D+03	0.7209223D+03	0.7040792D+03	0.6871353D+03
0.6700965D+03	0.6529699D+03	0.6357625D+03	0.6184822D+03
0.6011371D+03	0.5837364D+03	0.5662905D+03	0.5488067D+03
0.5312971D+03	0.5137733D+03	0.4962466D+03	0.4787299D+03
0.4612372D+03	0.4437817D+03	0.4263786D+03	0.4090435D+03
0.3917931D+03	0.3746439D+03	0.3576140D+03	0.3407227D+03
0.3239881D+03	0.3074313D+03	0.2910735D+03	0.2749349D+03
0.2590385D+03	0.2434088D+03	0.2280650D+03	0.2205088D+03
0.2130329D+03	0.2056408D+03	0.1983355D+03	0.1911205D+03
0.1839978D+03	0.1769712D+03	0.1700433D+03	0.1632169D+03
0.1564952D+03	0.1498812D+03	0.1433777D+03	0.1369917D+03
0.1307181D+03	0.1245637D+03	0.1185310D+03	0.1126229D+03
0.1068419D+03	0.1011918D+03	0.9567275D+02	0.9028818D+02
0.8504075D+02	0.7993258D+02	0.7496592D+02	0.7014285D+02
0.6546544D+02	0.6093566D+02	0.5655530D+02	0.5232642D+02
0.4825071D+02	0.4432990D+02	0.4056571D+02	0.3695975D+02
0.3351387D+02	0.3022968D+02	0.2710883D+02	0.2415319D+02
0.2136449D+02	0.1874450D+02	0.1629512D+02	0.1401819D+02
0.1191516D+02	0.9988402D+01	0.8238985D+01	0.6667964D+01
0.5275779D+01	0.4061974D+01	0.3024813D+01	0.2160805D+01
0.1464112D+01	0.9258662D+00	0.5334039D+00	0.2695375D+00
0.1120763D+00	0.3409850D-01	0.5944564D-02	0.3225429D-03
0.6984940D-06			
80HGL			
89			
0.6647545D+03	0.6493258D+03	0.6338125D+03	0.6182202D+03
0.6025552D+03	0.5868240D+03	0.5710335D+03	0.5551913D+03
0.5393063D+03	0.5233844D+03	0.5074358D+03	0.4914701D+03
0.4754969D+03	0.4595269D+03	0.4435711D+03	0.4276417D+03
0.4117505D+03	0.3959105D+03	0.3801356D+03	0.3644395D+03
0.3488372D+03	0.3333442D+03	0.3179769D+03	0.3027514D+03
0.2876853D+03	0.2727970D+03	0.2581036D+03	0.2436262D+03
0.2293820D+03	0.2153908D+03	0.2016737D+03	0.1949239D+03
0.1882500D+03	0.1816553D+03	0.1751413D+03	0.1687113D+03
0.1623674D+03	0.1561121D+03	0.1499481D+03	0.1438780D+03
0.1379042D+03	0.1320327D+03	0.1262590D+03	0.1205890D+03
0.1150249D+03	0.1095691D+03	0.1042239D+03	0.9899262D+02
0.9387511D+02	0.8887468D+02	0.8399326D+02	0.7923308D+02
0.7459597D+02	0.7008378D+02	0.6569833D+02	0.6144136D+02
0.5731455D+02	0.5331945D+02	0.4945784D+02	0.4573116D+02
0.4214094D+02	0.3868864D+02	0.3537569D+02	0.3220371D+02
0.2917409D+02	0.2628829D+02	0.2354795D+02	0.2095459D+02
0.1850976D+02	0.1621515D+02	0.1407241D+02	0.1208281D+02
0.1024858D+02	0.8570763D+01	0.7050509D+01	0.5688550D+01
0.4484999D+01	0.3439089D+01	0.2548828D+01	0.1810577D+01
0.1218544D+01	0.7642013D+00	0.4356644D+00	0.2171292D+00
0.8857747D-01	0.2619790D-01	0.4361244D-02	0.2169198D-03
0.3817647D-06			
81TLL			
89			
0.5993313D+03	0.5851153D+03	0.5708337D+03	0.5564923D+03
0.5420968D+03	0.5276534D+03	0.5131704D+03	0.4986519D+03
0.4841068D+03	0.4695432D+03	0.4549689D+03	0.4403931D+03
0.4258249D+03	0.4112746D+03	0.3967518D+03	0.3822676D+03
0.3678330D+03	0.3534606D+03	0.3391618D+03	0.3249498D+03
0.3108385D+03	0.2968407D+03	0.2829716D+03	0.2692458D+03
0.2556793D+03	0.2422868D+03	0.2290869D+03	0.2160925D+03
0.2033222D+03	0.1907939D+03	0.1785236D+03	0.1724914D+03
0.1665299D+03	0.1606422D+03	0.1548296D+03	0.1490950D+03

A.3 PIXAN data files

0.1434402D+03	0.1378674D+03	0.1323788D+03	0.1269797D+03
0.1216660D+03	0.1164426D+03	0.1113118D+03	0.1062754D+03
0.1013355D+03	0.9649388D+02	0.9175367D+02	0.8711443D+02
0.8257895D+02	0.7814921D+02	0.7382681D+02	0.6961336D+02
0.6551048D+02	0.6151969D+02	0.5764249D+02	0.5388032D+02
0.5023449D+02	0.4670657D+02	0.4329779D+02	0.4000946D+02
0.3684288D+02	0.3379925D+02	0.3088002D+02	0.2808640D+02
0.2541964D+02	0.2288121D+02	0.2047240D+02	0.1819460D+02
0.1604928D+02	0.1403789D+02	0.1216186D+02	0.1042233D+02
0.8821174D+01	0.7359248D+01	0.6037413D+01	0.4856109D+01
0.3815166D+01	0.2913557D+01	0.2149096D+01	0.1518068D+01
0.1014795D+01	0.6311442D+00	0.3560306D+00	0.1749884D+00
0.7002082D-01	0.2012315D-01	0.3195900D-02	0.1454133D-03
0.2068430D-06			
82PBL			
89			
0.5404973D+03	0.5274079D+03	0.5142694D+03	0.5010873D+03
0.4878685D+03	0.4746162D+03	0.4613382D+03	0.4480411D+03
0.4347318D+03	0.4214177D+03	0.4081065D+03	0.3948070D+03
0.3815272D+03	0.3682761D+03	0.3550634D+03	0.3418992D+03
0.3287932D+03	0.3157565D+03	0.3028001D+03	0.2899360D+03
0.2771756D+03	0.2645317D+03	0.2520174D+03	0.2396453D+03
0.2274292D+03	0.2153848D+03	0.2035229D+03	0.1918595D+03
0.1804100D+03	0.1691881D+03	0.1582098D+03	0.1528165D+03
0.1474892D+03	0.1422303D+03	0.1370414D+03	0.1319244D+03
0.1268810D+03	0.1219132D+03	0.1170261D+03	0.1122149D+03
0.1074846D+03	0.1028369D+03	0.9827346D+02	0.9379595D+02
0.8940606D+02	0.8510633D+02	0.8089632D+02	0.7677844D+02
0.7275444D+02	0.6882561D+02	0.6499336D+02	0.6125905D+02
0.5762399D+02	0.5408946D+02	0.5065661D+02	0.4732685D+02
0.4410126D+02	0.4098100D+02	0.3796720D+02	0.3506100D+02
0.3226346D+02	0.2957583D+02	0.2699920D+02	0.2453470D+02
0.2218347D+02	0.1994682D+02	0.1782591D+02	0.1582204D+02
0.1393650D+02	0.1217057D+02	0.1052526D+02	0.9002334D+01
0.7602616D+01	0.6327020D+01	0.5176168D+01	0.4150255D+01
0.3248871D+01	0.2470784D+01	0.1813673D+01	0.1273798D+01
0.8456361D+00	0.5214725D+00	0.2909970D+00	0.1409949D+00
0.5530900D-01	0.1543194D-01	0.2334863D-02	0.9694364D-04
0.1109368D-06			
83BIL			
89			
0.4878131D+03	0.4757643D+03	0.4636817D+03	0.4515680D+03
0.4394296D+03	0.4272722D+03	0.4151020D+03	0.4029247D+03
0.3907472D+03	0.3785764D+03	0.3664198D+03	0.3542843D+03
0.3421784D+03	0.3301101D+03	0.3180885D+03	0.3061219D+03
0.2942201D+03	0.2823926D+03	0.2706499D+03	0.2590019D+03
0.2474595D+03	0.2360343D+03	0.2247369D+03	0.2135804D+03
0.2025753D+03	0.1917336D+03	0.1810683D+03	0.1705926D+03
0.1603182D+03	0.1502587D+03	0.1404265D+03	0.1355996D+03
0.1308343D+03	0.1261320D+03	0.1214946D+03	0.1169235D+03
0.1124233D+03	0.1079896D+03	0.1036268D+03	0.9933641D+02
0.9511984D+02	0.9097861D+02	0.8691409D+02	0.8292768D+02
0.7902163D+02	0.7519531D+02	0.7145120D+02	0.6779044D+02
0.6421425D+02	0.6072384D+02	0.5732035D+02	0.5400492D+02
0.5077865D+02	0.4764253D+02	0.4459778D+02	0.4164534D+02
0.3878621D+02	0.3602139D+02	0.3335186D+02	0.3077855D+02
0.2830259D+02	0.2592490D+02	0.2364649D+02	0.2146837D+02
0.1939169D+02	0.1741747D+02	0.1554686D+02	0.1378102D+02
0.1212107D+02	0.1056791D+02	0.9123190D+01	0.7787666D+01
0.6562255D+01	0.5447666D+01	0.4444305D+01	0.3552155D+01
0.2770607D+01	0.2098271D+01	0.1532737D+01	0.1070291D+01
0.7056041D+00	0.4313954D+00	0.2381117D+00	0.1137118D+00
0.4371508D-01	0.1183491D-01	0.1704106D-02	0.6443446D-04
0.5903948D-07			
84POL			
89			

A PIXAN PACKAGE

0.4393255D+03	0.4282602D+03	0.4171721D+03	0.4060660D+03
0.3949471D+03	0.3838203D+03	0.3726913D+03	0.3615660D+03
0.3504508D+03	0.3393516D+03	0.3282752D+03	0.3172287D+03
0.3062196D+03	0.2952549D+03	0.2843426D+03	0.2734911D+03
0.2627090D+03	0.2520045D+03	0.2413868D+03	0.2308655D+03
0.2204503D+03	0.2101513D+03	0.1999771D+03	0.1899394D+03
0.1800476D+03	0.1703132D+03	0.1607464D+03	0.1513588D+03
0.1421604D+03	0.1331631D+03	0.1243771D+03	0.1200668D+03
0.1158134D+03	0.1116184D+03	0.1074857D+03	0.1034113D+03
0.9939916D+02	0.9545043D+02	0.9156649D+02	0.8774856D+02
0.8399784D+02	0.8031553D+02	0.7670364D+02	0.7316154D+02
0.6969142D+02	0.6629425D+02	0.6297113D+02	0.5972308D+02
0.5655114D+02	0.5345627D+02	0.5043947D+02	0.4750157D+02
0.4464369D+02	0.4186662D+02	0.3917126D+02	0.3655849D+02
0.3402916D+02	0.3158407D+02	0.2922423D+02	0.2695042D+02
0.2476352D+02	0.2266438D+02	0.2065401D+02	0.1873330D+02
0.1690318D+02	0.1516469D+02	0.1351880D+02	0.1196656D+02
0.1050873D+02	0.9146829D+01	0.7881545D+01	0.6713753D+01
0.5644180D+01	0.4673343D+01	0.3801450D+01	0.3028290D+01
0.2353087D+01	0.1774324D+01	0.1289536D+01	0.8950718D+00
0.5858281D+00	0.3549746D+00	0.1937097D+00	0.9112039D-01
0.3429947D-01	0.8997804D-02	0.1230185D-02	0.4218193D-04
0.3064662D-07			
86RNL			
89			
0.3581018D+03	0.3487583D+03	0.3394104D+03	0.3300622D+03
0.3207184D+03	0.3113836D+03	0.3020622D+03	0.2927594D+03
0.2834805D+03	0.2742310D+03	0.2650162D+03	0.2558420D+03
0.2467145D+03	0.2376402D+03	0.2286250D+03	0.2196759D+03
0.2107997D+03	0.2020036D+03	0.1932951D+03	0.1846803D+03
0.1761677D+03	0.1677644D+03	0.1594785D+03	0.1513184D+03
0.1432912D+03	0.1354057D+03	0.1276694D+03	0.1200909D+03
0.1126780D+03	0.1054386D+03	0.9838331D+02	0.9492512D+02
0.9151522D+02	0.8815464D+02	0.8484429D+02	0.8158509D+02
0.7837797D+02	0.7522381D+02	0.7212353D+02	0.6907870D+02
0.6608862D+02	0.6315508D+02	0.6027878D+02	0.5746052D+02
0.5470111D+02	0.5200129D+02	0.4936182D+02	0.4678344D+02
0.4426686D+02	0.4181271D+02	0.3942184D+02	0.3709486D+02
0.3483242D+02	0.3263521D+02	0.3050389D+02	0.2843906D+02
0.2644151D+02	0.2451185D+02	0.2265077D+02	0.2085893D+02
0.1913713D+02	0.1748605D+02	0.1590643D+02	0.1439909D+02
0.1296480D+02	0.1160438D+02	0.1031842D+02	0.9108202D+01
0.7974280D+01	0.6917419D+01	0.5938311D+01	0.5037539D+01
0.4215529D+01	0.3472484D+01	0.2808310D+01	0.2222512D+01
0.1714088D+01	0.1281383D+01	0.9219403D+00	0.6323204D+00
0.4079184D+00	0.2427850D+00	0.1294883D+00	0.5908299D-01
0.2131066D-01	0.5243762D-02	0.6451921D-03	0.1813663D-04
0.8225368D-08			
88RAL			
89			
0.2867758D+03	0.2790226D+03	0.2712782D+03	0.2635464D+03
0.2558309D+03	0.2481357D+03	0.2404649D+03	0.2328222D+03
0.2252122D+03	0.2176392D+03	0.2101082D+03	0.2026234D+03
0.1951905D+03	0.1878132D+03	0.1804976D+03	0.1732483D+03
0.1660710D+03	0.1589711D+03	0.1519546D+03	0.1450263D+03
0.1381925D+03	0.1314593D+03	0.1248319D+03	0.1183168D+03
0.1119194D+03	0.1056459D+03	0.9950194D+02	0.9349353D+02
0.8762662D+02	0.8190901D+02	0.7634200D+02	0.7361748D+02
0.7093318D+02	0.6828975D+02	0.6568786D+02	0.6312814D+02
0.6061113D+02	0.5813824D+02	0.5570875D+02	0.5332388D+02
0.5098420D+02	0.4869029D+02	0.4644270D+02	0.4424198D+02
0.4208865D+02	0.3998323D+02	0.3792617D+02	0.3591811D+02
0.3395948D+02	0.3205075D+02	0.3019241D+02	0.2838494D+02
0.2662882D+02	0.2492447D+02	0.2327248D+02	0.2167329D+02
0.2012738D+02	0.1863523D+02	0.1719743D+02	0.1581447D+02
0.1448689D+02	0.1321528D+02	0.1200020D+02	0.1084227D+02

A.3 PIXAN data files

0.9741891D+01	0.8700069D+01	0.7717215D+01	0.6793928D+01
0.5930778D+01	0.5128287D+01	0.4386900D+01	0.3706951D+01
0.3088622D+01	0.2531893D+01	0.2036471D+01	0.1601723D+01
0.1226581D+01	0.9094410D+00	0.6480495D+00	0.4393764D+00
0.2794903D+00	0.1634456D+00	0.8521318D-01	0.3770998D-01
0.1302533D-01	0.3001846D-02	0.3313803D-03	0.7593054D-05
0.2111548D-08			
90THL			
89			
0.2390094D+03	0.2323816D+03	0.2257704D+03	0.2191784D+03
0.2126091D+03	0.2060657D+03	0.1995515D+03	0.1930704D+03
0.1866254D+03	0.1802206D+03	0.1738596D+03	0.1675472D+03
0.1612856D+03	0.1550798D+03	0.1489339D+03	0.1428524D+03
0.1368390D+03	0.1308983D+03	0.1250350D+03	0.1192531D+03
0.1135574D+03	0.1079520D+03	0.1024418D+03	0.9703113D+02
0.9172443D+02	0.8652617D+02	0.8144100D+02	0.7647510D+02
0.7162897D+02	0.6690874D+02	0.6231850D+02	0.6007341D+02
0.5786224D+02	0.5568564D+02	0.5354453D+02	0.5143833D+02
0.4936804D+02	0.4733410D+02	0.4533698D+02	0.4337710D+02
0.4145490D+02	0.3957081D+02	0.3772525D+02	0.3591856D+02
0.3415130D+02	0.3242379D+02	0.3073644D+02	0.2908965D+02
0.2748382D+02	0.2591935D+02	0.2439659D+02	0.2291605D+02
0.2147809D+02	0.2008312D+02	0.1873157D+02	0.1742384D+02
0.1616046D+02	0.1494184D+02	0.1376843D+02	0.1264076D+02
0.1155932D+02	0.1052461D+02	0.9536993D+01	0.8597341D+01
0.7706006D+01	0.6863511D+01	0.6070368D+01	0.5327055D+01
0.4634009D+01	0.3991602D+01	0.3400114D+01	0.2859703D+01
0.2370368D+01	0.1931903D+01	0.1543845D+01	0.1205412D+01
0.9154298D+00	0.6722592D+00	0.4737062D+00	0.3169363D+00
0.1983917D+00	0.1137280D+00	0.5779663D-01	0.2472029D-01
0.8139906D-02	0.1746154D-02	0.1713422D-03	0.3150037D-05
0.5149831D-09			
92UL			
89			
0.1962955D+03	0.1907131D+03	0.1851518D+03	0.1796144D+03
0.1741032D+03	0.1686209D+03	0.1631706D+03	0.1577554D+03
0.1523775D+03	0.1470401D+03	0.1417463D+03	0.1364993D+03
0.1313024D+03	0.1261584D+03	0.1210708D+03	0.1160432D+03
0.1110784D+03	0.1061799D+03	0.1013515D+03	0.9659609D+02
0.9191740D+02	0.8731860D+02	0.8280307D+02	0.7837441D+02
0.7403751D+02	0.6979245D+02	0.6564408D+02	0.6159559D+02
0.5765014D+02	0.5381081D+02	0.5008052D+02	0.4825769D+02
0.4646278D+02	0.4469659D+02	0.4295947D+02	0.4125176D+02
0.3957379D+02	0.3792591D+02	0.3630844D+02	0.3472165D+02
0.3316598D+02	0.3164168D+02	0.3014907D+02	0.2868848D+02
0.2726020D+02	0.2586455D+02	0.2450186D+02	0.2317238D+02
0.2187653D+02	0.2061458D+02	0.1938688D+02	0.1819373D+02
0.1703550D+02	0.1591250D+02	0.1482514D+02	0.1377378D+02
0.1275876D+02	0.1178052D+02	0.1083944D+02	0.9935938D+01
0.9070284D+01	0.8243213D+01	0.7454998D+01	0.6706072D+01
0.5996859D+01	0.5327771D+01	0.4699195D+01	0.4111482D+01
0.3564931D+01	0.3059773D+01	0.2596145D+01	0.2174066D+01
0.1793404D+01	0.1453840D+01	0.1154826D+01	0.8955328D+00
0.6748033D+00	0.4910879D+00	0.3423854D+00	0.2261829D+00
0.1394032D+00	0.7837399D-01	0.3884021D-01	0.1605928D-01
0.5040611D-02	0.1005884D-02	0.8765618D-04	0.1290430D-05
0.1218784D-09			
94PUL			
89			
0.1617548D+03	0.1570514D+03	0.1523719D+03	0.1477175D+03
0.1430909D+03	0.1384944D+03	0.1339300D+03	0.1294002D+03
0.1249072D+03	0.1204538D+03	0.1160419D+03	0.1116742D+03
0.1073533D+03	0.1030818D+03	0.9886187D+02	0.9469648D+02
0.9058783D+02	0.8653882D+02	0.8255182D+02	0.7862948D+02
0.7477433D+02	0.7098909D+02	0.6727771D+02	0.6363982D+02
0.6007932D+02	0.5659864D+02	0.5320019D+02	0.4988635D+02

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0.4665936D+02	0.4352198D+02	0.4047559D+02	0.3898733D+02
0.3752272D+02	0.3608201D+02	0.3466547D+02	0.3327336D+02
0.3190586D+02	0.3056334D+02	0.2924600D+02	0.2795408D+02
0.2668782D+02	0.2544749D+02	0.2423332D+02	0.2304556D+02
0.2188446D+02	0.2075023D+02	0.1964322D+02	0.1856364D+02
0.1751175D+02	0.1648782D+02	0.1549210D+02	0.1452494D+02
0.1358659D+02	0.1267735D+02	0.1179751D+02	0.1094742D+02
0.1012739D+02	0.9337631D+01	0.8578752D+01	0.7850959D+01
0.7154605D+01	0.6490044D+01	0.5857629D+01	0.5257705D+01
0.4690607D+01	0.4156647D+01	0.3656108D+01	0.3189235D+01
0.2756216D+01	0.2357169D+01	0.1992124D+01	0.1660996D+01
0.1363565D+01	0.1099443D+01	0.8680389D+00	0.6685245D+00
0.4997918D+00	0.3604102D+00	0.2485829D+00	0.1621065D+00
0.9834032D-01	0.5419694D-01	0.2617249D-01	0.1044997D-01
0.3121463D-02	0.5780345D-03	0.4455534D-04	0.5216464D-06
0.2747841D-10			
95 AML			
89			
0.1465408D+03	0.1422327D+03	0.1379487D+03	0.1336908D+03
0.1294607D+03	0.1252605D+03	0.1210922D+03	0.1169582D+03
0.1128601D+03	0.1088002D+03	0.1047808D+03	0.1008042D+03
0.9687224D+02	0.9298732D+02	0.8915186D+02	0.8536773D+02
0.8163753D+02	0.7796330D+02	0.7434731D+02	0.7079180D+02
0.6729912D+02	0.6387282D+02	0.6051237D+02	0.5722126D+02
0.5400163D+02	0.5085557D+02	0.4778516D+02	0.4479234D+02
0.4187957D+02	0.3904801D+02	0.3629992D+02	0.3495774D+02
0.3363713D+02	0.3233829D+02	0.3106146D+02	0.2980679D+02
0.2857463D+02	0.2736513D+02	0.2617851D+02	0.2501500D+02
0.2387480D+02	0.2275813D+02	0.2166523D+02	0.2059626D+02
0.1955154D+02	0.1853125D+02	0.1753562D+02	0.1656489D+02
0.1561930D+02	0.1469907D+02	0.1380451D+02	0.1293584D+02
0.1209334D+02	0.1127727D+02	0.1048794D+02	0.9725612D+01
0.8990480D+01	0.8283103D+01	0.7603656D+01	0.6952455D+01
0.6329816D+01	0.5736057D+01	0.5171490D+01	0.4636417D+01
0.4131127D+01	0.36555886D+01	0.3210926D+01	0.2796440D+01
0.2412566D+01	0.2059372D+01	0.1736839D+01	0.1444841D+01
0.1183120D+01	0.9512639D+00	0.7486725D+00	0.5745268D+00
0.4277543D+00	0.3069917D+00	0.2105490D+00	0.1363776D+00
0.8204761D-01	0.4474669D-01	0.2131631D-01	0.8355457D-02
0.2431243D-02	0.4327166D-03	0.3124791D-04	0.3236103D-06
0.1237676D-10			
96 CML			
89			
0.1331415D+03	0.1291894D+03	0.1252613D+03	0.1213592D+03
0.1174848D+03	0.1136399D+03	0.1098265D+03	0.1060460D+03
0.1023007D+03	0.9859238D+02	0.9492310D+02	0.9129444D+02
0.8770854D+02	0.8416750D+02	0.8067301D+02	0.7722729D+02
0.7383213D+02	0.7048945D+02	0.6720139D+02	0.6396987D+02
0.6079809D+02	0.5768543D+02	0.5463501D+02	0.5164872D+02
0.4872839D+02	0.4587584D+02	0.4309278D+02	0.4038140D+02
0.3774267D+02	0.3517861D+02	0.3269084D+02	0.3147606D+02
0.3028096D+02	0.2910568D+02	0.2795052D+02	0.2681562D+02
0.2570116D+02	0.2460736D+02	0.2353440D+02	0.2248247D+02
0.2145177D+02	0.2044250D+02	0.1945482D+02	0.1848900D+02
0.1754522D+02	0.1662367D+02	0.1572458D+02	0.1484816D+02
0.1399460D+02	0.1316419D+02	0.1235713D+02	0.1157367D+02
0.1081404D+02	0.1007851D+02	0.9367347D+01	0.8680694D+01
0.8019071D+01	0.7382632D+01	0.6771662D+01	0.6186447D+01
0.5627275D+01	0.5094429D+01	0.4588187D+01	0.4108816D+01
0.3656565D+01	0.3231658D+01	0.2834288D+01	0.2464604D+01
0.2122702D+01	0.1808611D+01	0.1522272D+01	0.1263528D+01
0.1032097D+01	0.8275501D+00	0.6492863D+00	0.4965033D+00
0.3681678D+00	0.2629840D+00	0.1793637D+00	0.1154011D+00
0.6885695D-01	0.3716342D-01	0.1746497D-01	0.6721071D-02
0.1905259D-02	0.3259989D-03	0.2206971D-04	0.2024472D-06
0.5608320D-11			

61PML				
89				
0.4823754D+04	0.4764327D+04	0.4703328D+04	0.4640714D+04	
0.4576488D+04	0.4510606D+04	0.4443042D+04	0.4373758D+04	
0.4302755D+04	0.4229997D+04	0.4155461D+04	0.4079118D+04	
0.4000963D+04	0.3920981D+04	0.3839153D+04	0.3755469D+04	
0.3669921D+04	0.3582509D+04	0.3493231D+04	0.3402095D+04	
0.3309114D+04	0.3214305D+04	0.3117696D+04	0.3019319D+04	
0.2919219D+04	0.2817448D+04	0.2714070D+04	0.2609163D+04	
0.2502818D+04	0.2395142D+04	0.2286257D+04	0.2231406D+04	
0.2176307D+04	0.2120982D+04	0.2065454D+04	0.2009746D+04	
0.1953884D+04	0.1897895D+04	0.1841807D+04	0.1785651D+04	
0.1729459D+04	0.1673266D+04	0.1617106D+04	0.1561019D+04	
0.1505051D+04	0.1449231D+04	0.1393608D+04	0.1338229D+04	
0.1283145D+04	0.1228403D+04	0.1174057D+04	0.1120163D+04	
0.1066779D+04	0.1013962D+04	0.9617731D+03	0.9102790D+03	
0.8595406D+03	0.8096264D+03	0.7606073D+03	0.7125473D+03	
0.6655223D+03	0.6195982D+03	0.5748575D+03	0.5313565D+03	
0.4891697D+03	0.4483688D+03	0.4090389D+03	0.3712126D+03	
0.3349750D+03	0.3003742D+03	0.2674728D+03	0.2363228D+03	
0.2069715D+03	0.1794628D+03	0.1538344D+03	0.1301204D+03	
0.1083512D+03	0.8855364D+02	0.7075274D+02	0.5497110D+02	
0.4122982D+02	0.2954582D+02	0.1992543D+02	0.1235768D+02	
0.6787984D+01	0.3090812D+01	0.1023682D+01	0.1813968D+00	
0.6535065D-02				
63EUL				
89				
0.3897626D+04	0.3844796D+04	0.3790721D+04	0.3735374D+04	
0.3678758D+04	0.3620848D+04	0.3561621D+04	0.3501078D+04	
0.3439197D+04	0.3375973D+04	0.3311393D+04	0.3245449D+04	
0.3178137D+04	0.3109454D+04	0.3039399D+04	0.2967974D+04	
0.2895186D+04	0.2821045D+04	0.2745565D+04	0.2668764D+04	
0.2590667D+04	0.2511303D+04	0.2430708D+04	0.2348925D+04	
0.2266005D+04	0.2182008D+04	0.2097002D+04	0.2011067D+04	
0.1924293D+04	0.1836783D+04	0.1748653D+04	0.1704396D+04	
0.1660034D+04	0.1615587D+04	0.1571073D+04	0.1526515D+04	
0.1481933D+04	0.1437352D+04	0.1392796D+04	0.1348290D+04	
0.1303867D+04	0.1259545D+04	0.1215357D+04	0.1171334D+04	
0.1127510D+04	0.1083919D+04	0.1040593D+04	0.9975705D+03	
0.9548904D+03	0.9125880D+03	0.8707057D+03	0.8292850D+03	
0.7883702D+03	0.7480021D+03	0.7082271D+03	0.6690932D+03	
0.6306431D+03	0.5929283D+03	0.5559923D+03	0.5198926D+03	
0.4846644D+03	0.4503607D+03	0.4170291D+03	0.3847175D+03	
0.3534854D+03	0.3233495D+03	0.2943711D+03	0.2665814D+03	
0.2400239D+03	0.2147349D+03	0.1907473D+03	0.1680927D+03	
0.1467981D+03	0.1268886D+03	0.1083870D+03	0.9131324D+02	
0.7568577D+02	0.6152220D+02	0.4883858D+02	0.3765034D+02	
0.2797074D+02	0.1980707D+02	0.1315919D+02	0.8003772D+01	
0.4282682D+01	0.1878845D+01	0.5874997D+00	0.9396484D-01	
0.2672518D-02				

B ptanal

The PIGE analysis of this package is based on [ptanal](#), a peak finding package developed at ANSTO. [ptanal](#) is a search routine that finds peaks in a spectrum and reports on the energy and channel number of the peak as well as peak area, background area, total area, error and peak resolution. To get the energy of the peak, an energy calibration is required as input. The operation of [ptanal](#) is controlled by a run control file.

PTANAL run control file

The [ptanal](#) run control file has a fixed format. [ptanal](#) is a very flexible program and there are many different ways to set for instance the energy calibration. The example of a run control file shown below, is of the type created by [doiba](#) to run [ptanal](#).

Example of [ptanal](#) run control file

```
resetn 2048
plotdev "screen"
calib 0.0040085 (-0.0035242)
for ( i = 3131; i <= 3131; i=i+1) {
    getf "/home/usr/analysis/pige/pige031.rpt" 1 i
    peakfind 1 40 4 2 1 1
    sum 1 1251 1801
    sum 1 1851 1951
}
```

Line 1: This first line resets the number of channels to 2048. For larger spectra sizes this has be changed appropriately.

Line 2: This defines the plotting device.

Line 3: The next line set the energy calibration, with slope and offset. A negative offset has to be written in brackets.

Line 4: The `for` loop repeats the command in the curly brackets, for all the block numbers that fulfill the condition of the loop.

Line 5: The first line in the loop is the command to open the file and access the block i in the file.

Line 6: The `peakfind` routine analysis the each spectrum for peaks using the the parameters that follow.

Line 7+8: The next two line sum the spectra from the minimum to maximum channel number.

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