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Rev. 1

INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

IMPLEMENTING AND TESTING

PROGRAM PLOTTAB

by

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Abstract: Enclosed is a description of the magnetic tape or floppy diskette containing the PLOTTAB code package. In addition detailed information is provided on implementation and testing of this code. See part I for mainframe computers; part II for personal computers. These codes are documented in IAEA-NDS-82.

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SUMMARY OF PROGRAM PLOTTAB (VERSION 87-2)

PURPOSE

THIS PROGRAM IS DESIGNED TO PLOT ANY COMBINATION OF CONTINUOUS CURVES AND/OR DISCRETE POINTS (WITH ASSOCIATED ERROR BARS) USING USER SUPPLIED TITLES AND X AND Y AXIS LABELS AND UNITS.

USING THIS METHOD THE PROGRAM HAS NO IDEA OF WHAT DATA IS BEING PLOTTED AND YET BY SUPPLYING TITLES, X AND Y AXIS LABELS AND UNITS THE USER CAN PRODUCE ANY NUMBER OF PLOTS WITH EACH PLOT CONTAINING ANY COMBINATION OF CURVES AND POINTS WITH EACH PLOT PROPERLY IDENTIFIED.

GRAPHICS INTERFACE

THIS PROGRAM USES A SIMPLE CALCOMP LIKE GRAPHICS INTERFACE WHICH REQUIRES ONLY 3 SUBROUTINES...PLOTS, PLOT AND PEN (DESCRIBED IN THE PROGRAM DOCUMENTATION). ALL CHARACTERS AND SYMBOLS ARE DRAWN USING TABLES OF PEN STROKES (SUPPLIED WITH THIS PROGRAM). USING THIS METHOD THE PROGRAM SHOULD BE SIMPLE TO INTERFACE TO VIRTUALLY ANY PLOTTER OR GRAPHICS TERMINAL AND THE APPEARANCE AND LAYOUT OF THE PLOTS SHOULD BE INDEPENDENT OF WHICH PLOTTER IS USED.

CODE	VERSION	CPU TIME	CORE (KILO BYTES)	PURPOSE
PLOTTAB	87-2	0.04	456	PLOT ANY COMBINATION OF CURVES AND/OR POINTS

CPU TIME = IBM-3083 CPU MINUTES FOR ENCLOSED EXAMPLE PROBLEM.
CORE = IBM FORTRAN-77 COMPILER

COMPUTERS ON WHICH PROGRAM WILL OPERATE

THIS PROGRAM IS DESIGNED TO OPERATE ON VIRTUALLY ANY TYPE OF COMPUTER FROM LARGE MAINFRAMES ALL THE WAY DOWN TO AN IBM-PC-AT. THE REMAINDER OF THIS REPORT DESCRIBES THE PROGRAM AS IMPLEMENTED ON A MAINFRAME COMPUTER. CONTACT THE AUTHOR IF YOU WISH TO OBTAIN A COPY OF THIS PROGRAM ON DISKETTES FOR USE ON AN IBM-PC-AT (WARNING...THIS PROGRAM ON DISKETTES IS ONLY DISTRIBUTED ON 1.2 MEGABYTE DISKETTES WHICH CAN ONLY BE USED ON A PC WITH 1.2 MEGABYTE DISK DRIVES, E.G. AN IBM-PC-AT. PLEASE DO NOT REQUEST THIS PROGRAM ON DISKETTES IF YOU HAVE A NORMAL IBM-PC OR AN IBM-PC-XT, SINCE THESE PC DO NOT HAVE 1.2 MEGABYTE DISK DRIVES).

PLOTTER ON WHICH PROGRAM WILL OPERATE

THIS PROGRAM HAS A SIMPLE CALCOMP LIKE INTERFACE TO WHICHEVER PLOTTER IS USED. THE INTERFACE CONSISTS OF ONLY 3 SUBROUTINES...PLOTS, PLOT AND PEN. ALL CHARACTERS AND SYMBOLS ARE DRAWN USING SOFTWARE CONTROLLED TABLES CONTAINING X AND Y COORDINATES AND PEN POSITIONS WHICH ARE COMPLETELY PLOTTER INDEPENDENT. USING THESE CONVENTIONS THIS PROGRAM CAN BE INTERFACED TO USE ALMOST ANY PLOTTER OR GRAPHICS TERMINAL (SEE, PROGRAM PLOTTAB DOCUMENTATION FOR DETAILS).

FORMAT OF CODES AS DISTRIBUTED

THIS CODE REQUIRES A FORTRAN-77 COMPILER AND A SIMPLE CALCOMP LIKE GRAPHICS INTERFACE (FOR DETAILS SEE DOCUMENTATION OF PROGRAM PLOTTAB).

SUMMARY OF CONTENTS OF THE PLOTTAB TAPE

THE PLOTTAB CODE PACKAGE CONSISTS OF A MAGNETIC TAPE CONTAINING 9 FILES OF INFORMATION.

TAPE FILE	DESCRIPTION
1	FORTRAN PROGRAM
2	SUBROUTINE PEN (DUMMY) (*)
3	SOFTWARE CHARACTER TABLE (*)
4	STANDARD SYMBOL AND LINE TYPE TABLE (*)
5	ALTERNATE SYMBOL AND LINE TYPE TABLE (*)
6	JOB CONTROL LANGUAGE AND INPUT PARAMETERS (BATCH DECK TO EXECUTE PROGRAM AND PRODUCE PLOTS)
7	DATA FOR CURVES
8	DATA FOR DISCRETE POINTS
9	OUTPUT REPORT

(*) FOR DETAILS SEE PROGRAM PLOTTAB DOCUMENTATION.

FILES 1 THROUGH 8 HAVE 80 CHARACTERS PER RECORD.
FILE 9 HAS 132 CHARACTERS PER RECORD.

IMPLEMENTING AND TESTING CODES

THE INPUT PARAMETERS SUPPLIED FOR THIS CODE ARE DESIGNED TO OPERATE ON THE INDICATED DATA AND TO PRODUCE THE OUTPUT REPORT INCLUDED ON THE PLOTTAB TAPE AND THE PLOTS INCLUDED IN THE DOCUMENTATION FOR PROGRAM PLOTTAB.

IN ORDER TO IMPLEMENT AND TEST THIS CODE IT IS SUGGESTED THAT THE USER,
(1) COMPILE AND LOAD THE PROGRAM
(2) EXECUTE THE PROGRAM USING THE INPUT PARAMETERS AND DATA SUPPLIED WITH THIS CODE PACKAGE.
(3) COMPARE THE RESULTS OBTAINED TO THE TEST RESULTS INCLUDED IN THIS CODE PACKAGE.

COMPILING AND CREATING LOAD MODULES ON IBM COMPUTERS

THE FOLLOWING JCL DECK ILLUSTRATES HOW TO COMPILE THE PROGRAM AND CREATE A LOAD MODULE ON AN IBM COMPUTER. (1) A DUMMY SUBROUTINE PEN HAS BEEN CONCATENATED TO THE PROGRAM DURING COMPILATION TO PRODUCE BLACK-WHITE PLOTS (IGNOR ATTEMPTS TO CHANGE COLOR). (2) THE PROGRAM IS LINKED TO TO THE GRAPHICS SOFTWARE AVAILABLE AT IAEA TO PRODUCE PLOTS ON A BENSON-VARIAN PLOTTER (THIS PROCEDURE MAY DIFFER AT OTHER INSTALLATIONS).

EXAMPLE

```
//RNC1  JOB (NO,T),A2323-CULLEN,CLASS=I,MSGCLASS=X,NOTIFY=RNC,
//  TIME=(1,00)
//PASS1  EXEC  FORTCL,
//       LOADLIB='XNDC.EVALLIB',
//     DISP=SHR,
//       MEMBER=PLOTTAB
//FORT.SYSLIN DD SPACE=(800,(160,100))
//FORT.SYSIN   DD  DSN=XNDC.PLOTTAB.SEND(PLOTTAB),DISP=SHR
//             DD  DSN=XNDC.PLOTTAB.SEND(PEN),DISP=SHR
//LKED.SYSUT1  DD  SPACE=(1024,(800,300),RLSE)
//LKED.GR  DD  DSN=XCSX.VARIAN.LOAD,DISP=SHR
//LKED.SYSIN  DD  *
 INCLUDE GR(GRAPHICS)
//
```

REPORTING ERRORS

WE ARE ATTEMPTING TO MAKE THIS CODE AS COMPATIBLE AS POSSIBLE FOR USE WITH AS MANY DIFFERENT COMPUTERS AS POSSIBLE. IN ORDER TO HELP US AND TO INSURE THAT FUTURE VERSIONS OF THIS CODE ARE AS COMPATIBLE AS POSSIBLE FOR USE AT YOUR INSTALLATION PLEASE REPORT ANY (REPEAT, ANY) COMPILER, LOADER OR EXECUTION DIAGNOSTICS OR PROBLEMS TO THE AUTHOR.

PLEASE REMEMBER IF YOU SIMPLY REPORT 'I'VE GOT A PROBLEM' AND DO NOT ADEQUATELY DESCRIBE EXACTLY HOW YOU WERE USING THE PROGRAM IT WILL BE IMPOSSIBLE FOR THE AUTHOR TO HELP YOU. WHEN A PROBLEM ARISES PLEASE WRITE TO THE AUTHOR, DESCRIBE THE PROBLEM IN AS MUCH DETAIL AS POSSIBLE, IDENTIFY THE VERSION OF THE PROGRAM (E.G. VERSION 86-1) THAT YOU ARE USING AND SEND THE FOLLOWING INFORMATION ON MAGNETIC TAPE TO THE AUTHOR,

(1) A COPY OF THE PROGRAM YOU ARE USING
(2) A COPY OF THE SOFTWARE CHARACTER TABLE
(3) A COPY OF THE SOFTWARE SYMBOL TABLE
(4) A COPY OF COMPILER DIAGNOSTICS (IF ANY)
(5) A COPY OF THE JCL DECK YOU USED TO EXECUTE THE PROGRAM
(6) A COPY OF THE CURVE DATA
(7) A COPY OF THE DISCRETE POINT DATA
(8) A COPY OF THE OUTPUT REPORT FROM THE PROGRAM
(9) A COPY OF THE PLOTS

WITHOUT ALL OF THIS INFORMATION IT IS IMPOSSIBLE TO EXACTLY SIMULATE THE PROBLEM THAT YOU RAN AND TO DETERMINE THE SOURCE OF YOUR PROBLEM.

CODE DOCUMENTATION

THIS CODE IS DESIGNED TO BE SELF DOCUMENTING, IN THE SENSE THAT THE LATEST DOCUMENTATION FOR THE CODE INCLUDING A COMPLETE DESCRIPTION OF ALL INPUT PARAMETERS AND ASSIGNED INPUT/OUTPUT UNITS IS INCLUDED ON THE COMMENT CARDS AT THE BEGINNING OF THE CODE. PRINTED DOCUMENATION FOR THIS CODE IS PERIODICALLY PUBLISHED. MOST OF THIS DOCUMENTATION CONSISTS CONSISTS OF A COPY OF THE COMMENT CARDS FROM THE BEGINNING OF THE CODE. THE USER SHOULD BE AWARE THAT THE LATEST DOCUMENTATION IS ALWAYS THE THE COMMENT CARDS AT THE BEGINNING OF THE CODE (WHICH MAY SUPERSEDE THE MOST RECENT PRINTED DOCUMENTATION) AND THE USER SHOULD ALWAYS READ THE DOCUMENTATION IN THE CODE BEFORE USING THE CODE.

CONTENTS OF TAPE.

DISK FILENAMES DESCRIBED BELOW ONLY REFER TO THE CONVENTIONS USED AT THE NUCLEAR DATA SECTION, IAEA, VIENNA AND ARE ONLY INCLUDED BELOW FOR THE CONVENIENCE OF THE STAFF OF THE NUCLEAR DATA SECTION (I.E. THEY MAY BE IGNORED BY ALL OTHER PROGRAM USERS).

FILE	DESCRIPTION	RECORDS	RECORD LENGTH	DISK FILENAME XNDC.PLOTTAB.SEND
1	PROGRAM PLOTTAB	3863	80	PLOTTAB
2	SUBROUTINE PEN (DUMMY)	7	80	PEN
3	SOFTWARE CHARACTER TABLE	1468	80	CHARACTR
4	STANDARD SYMBOL/LINE TABLE	455	80	SYMBOLS1
5	ALTERNATE SYMBOL/LINE TABLE	516	80	SYMBOLS2
6	PLOTTAB JCL/INPUT PARAMETERS	33	80	GOPLOTTA
7	CURVE DATA	268	80	CURVES
8	POINT DATA	74	80	POINTS

FILE	DESCRIPTION	RECORDS	RECORD LENGTH	DISK FILENAME XNDC.PLOTTAB.REPORT
9	OUTPUT REPORT	135	132	PLOTTAB
	TAPE TOTAL RECORDS	6819		

PROGRAM PLOTTAB (VERSION 87-2)

Part II:Implementing and Testing on a Personal Computer

This document describes the contents of the diskette containing the PLOTTAB code package by D.E.Cullen and example data for use in implementing and testing these codes on a Personal computer of the type IBM-PC/AT. Upon request the codes are available from the IAEA Nuclear Data Section, free of charge, on a high density diskette.

The PLOTTAB code package by Dermott.E.Cullen are described in the document IAEA-NDS-82(Rev.0) of June 1987.
These codes are now available for a Personal Computer of the type IBM-PC/AT with a 1.2 Mbyte diskette drive. The present document describes the content of the diskette containing the PLOTTAB code, and gives instructions on how to implement and test the code on your Personal Computer.

Upon request, the diskette is available free of charge from the IAEA Nuclear Data Section, under the condition that all difficulties or defaults encountered are reported to the IAEA Nuclear Data Section. If results obtained from these codes are mentioned in a publication, a reprint is requested to be sent to the IAEA Nuclear Data Section.

Contents of the diskettes

Diskette No.	Contents
IAEA/NDS-D82/1	PLOTTAB.FOR
	PLOTPACK.FOR
	PLOTTAB.INP
	CHARACTR.DAT
	SYMBOLS1.TAB
	SYMBOLS2.TAB
	GOPLOTAB.BAT
	CURVES.DAT
	POINTS.BAT
	PLOTTAB.LST

Contents of this document

Summary of PLOTTAB codes for use on a Personal Computer

This code is designed to plot any combination of continuous curves and/or discreet points (with associated error bars) using user supplied titles and X and Y axis labels and units.

Codes in the order in which they are normally used

Code	Version	File size (Kbytes)	Purpose
PLOTTAB	87-2	317	Starting from any combination of continuous data and/or discrete points plot a comparison of up to 30 sets of tables and/or discrete points with associated error bars.
			Additional subroutine to be included at Compile/Link stage. See "Compiling and creating load modules on Personal Computers" below.
PLOTPACK		73	Graphics Interface for Hewlett-Packard 7475A plotter

Personal Computers on which codes will operate

These codes on diskette were developed for use on an IBM-PC-AT under the IBM Disk Operating System DOS-3.20 and require 512 Kilobytes of memory and a math co-processor. For practical use of these codes a hard disk drive is highly desirable. Compilation, linkage and execution is performed using the IBM Personal Computer Professional FORTRAN (PROFORT) by Ryan-McFarlane Corporation. The codes operate with Double Precision Arithmetic. The batch (BAT) files used for running the jobs may not conform with other PC operating systems and may need changes.

(WARNING...Codes on diskettes are only distributed on 1.2 Megabyte diskettes, which can only be used on a PC with 1.2 Megabyte disk drives, e.g. an IBM-PC-AT. Please do not request the codes on diskette if you have a normal IBM-PC or an IBM-PC-XT, since these PC's do not have 1.2 Megabyte disk drives).

Conversion for use on Computer/Compiler/Precision Combinations

As distributed for use on a personal Computer the codes are set up to use FORTRAN-77 conventions and DOUBLE PRECISION arithmetic.

Summary of contents of the PLOTTAB diskette

The PLOTTAB code package consists of one diskette containing 10 files of information. Six different types of files are included on the diskette.

Description	Type	Disk files
(1) FORTRAN codes (Source modules)	.FOR	2 files
(2) Batch (BAT) files (Job control language)	.BAT	1 files
(3) Input parameters	.INP	1 files
(4) Input/output data	.DAT	3 files
(5) Tables	.TAB	2 files
(6) Output reports	.LST	1 files

Implementing and testing codes

The input parameters supplied for each code are designed to operate on the indicated data and to produce the output reports included on this diskette.

For details of the input parameters see the report IAEA-NDS-82: 'Program PLOTTAB'.

In order to implement and test these codes it is suggested that the user,

(1) Compile (.FOR) and load each code,then execute (.BAT) using the Input (.INP) parameters and input data supplied with this code package. See "Compiling and creating load modules" below.

(2) Compare the Output reports with those included on the diskette.

The codes were implemented on the PC in the following order, the output from the first code being the input to the next code.

Code	Batch file	Code input	Code output	Report
PLOTTAB	GOPLOTAB.BAT	CURVES.DAT	Graphics	PLOTTAB.LST
PLOTPACK		POINTS.DAT		
		CHARACTR.DAT		
		SYMBOLS1.TAB		
		SYMBOLS2.TAB		

The input parameters for the code is in the .INP file.
e.g. PLOTTAB.INP.

Compiling and creating load modules on Personal Computers

Compilation and linking will vary from Operating Systems and Compilers depending on the configuration the user employs. As mentioned above this package was developed using IBM DOS-3.20 and the PROFORT Compiler of Ryan-McFarlane Corporation.

This package includes a graphics interface for a Hewlett-Packard 7475A plotter. If you have this plotter you may use the interface routines in PLOTPACK. If you do not, you must provide your own interface.
For PLOTTAB compile and include subroutine PLOTPACK at the LINK stage,
e.g.

```
PROFORT PLOTTAB /L > PLOTTAB.LST
PROFORT PLOTPACK /L > PLOTPACK.LST
LINK PLOTTAB+PLOTPACK;
```

Executing codes on Personal Computers

The code has a batch file which is used to define all input and output files, to execute the code and to delete all scratch files after execution. After a code has been compiled and loaded it may be executed by typing the name of the batch file (NOT execution module),e.g.GOPLOTAB.BAT

Below is an example of a BAT (Job control) file used for executing the code PLOTTAB. (Might vary from PC to PC)

```
SET FORT4  = PLOTTAB.INP  ..........  Input Parameters

SET FORT10 = CURVES.DAT   ..........  Input data

SET FORT11 = POINTS.DAT   ..........  Input data

SET FORT12 = CHARACTR.DAT ..........  Input data

SET FORT14 = SYMBOLS1.TAB ..........  Input table

PLOTTAB /R 41000 > PLOTTAB.LST   ...  Execute code,
                                      ... and write output report on
                                      ... PLOTTAB.LST.
```

The graphics output from code PLOTTAB was produced via the software interface PLOTPACK to a Hewlett Packard 7475A Plotter.See Output Reports.

Reporting errors

We are attempting to make these codes as compatible as possible for use with as many different Personal Computers as possible. In order to help us and to insure that future versions of these codes are as compatible as possible for use at your installation please report any (repeat, any) Compiler, Loader or execution diagnostics or problems to the author, describing the problem in as much detail as possible. Identify the version of the code (e.g. Version 87-1) that you are using and send the following information on diskette.

(1) A copy of the code you are using

(2) A copy of compiler diagnostics (if any)

(3) A copy of the JCL deck (BAT file) that executes the code

(4) A copy of the output report from the code

In addition for code PLOTTAB send,

(1) A copy of the software character table

(2) A copy of the software symbol table

(3) A copy of the curve data

(4) A copy of the discreet point data

(5) A copy of the plots

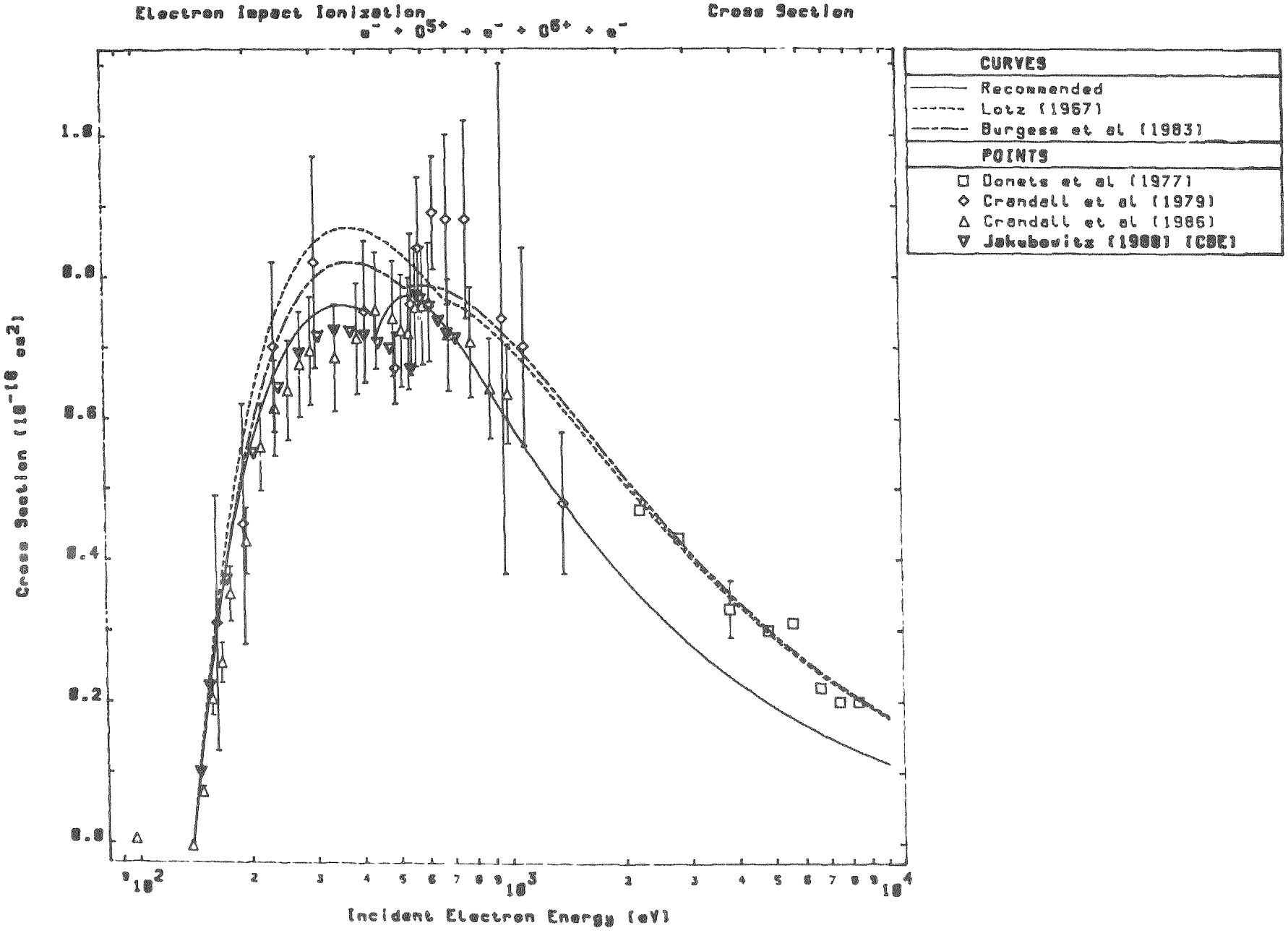
Without ALL of this information it is impossible to exactly simulate the problem that you ran and to determine the source of your problem.

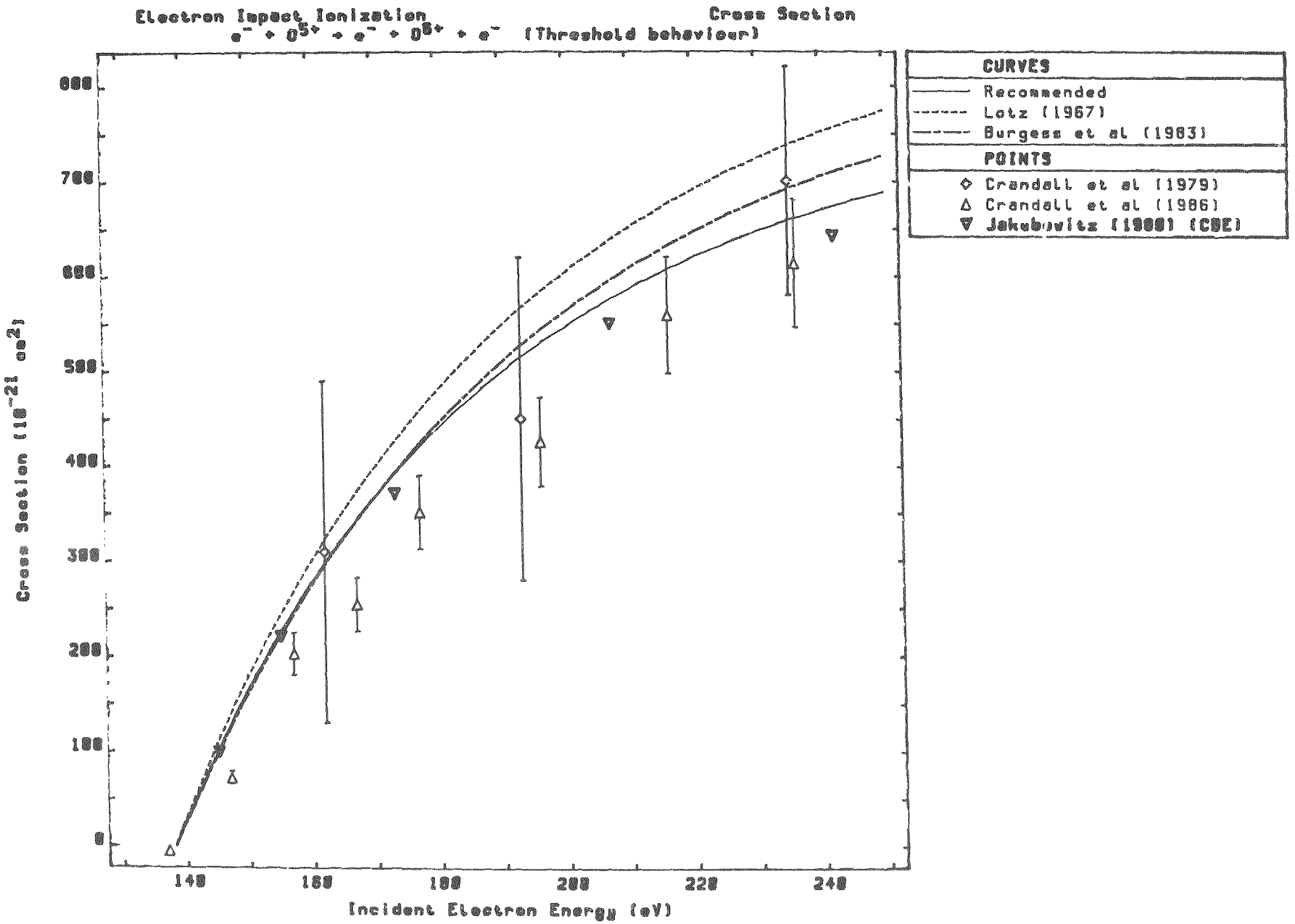
Code Documentation

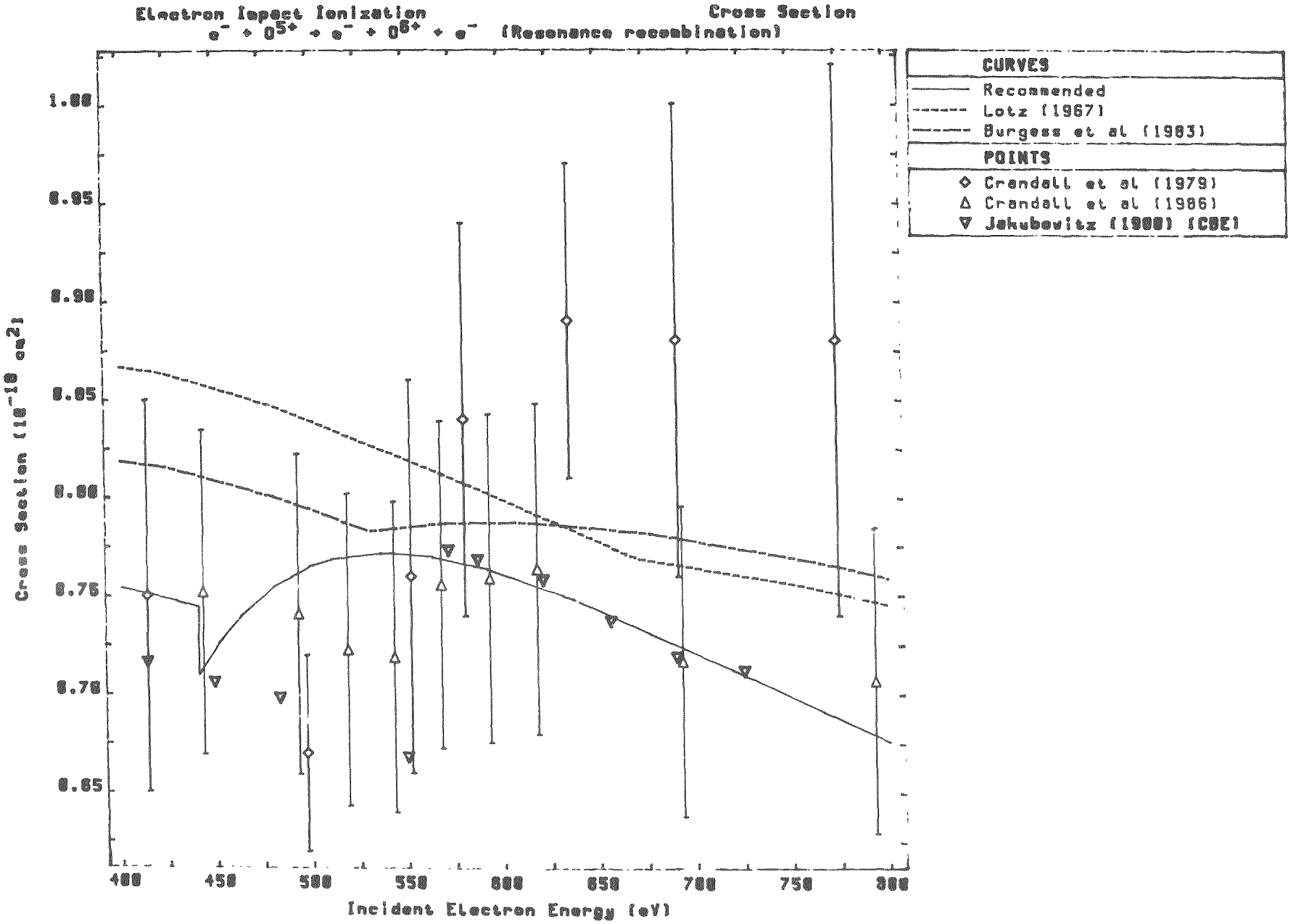
For details of the Code Documentation see the report IAEA-NDS-82
' PROGRAM PLOTTAB by Dermott.E.Cullen.

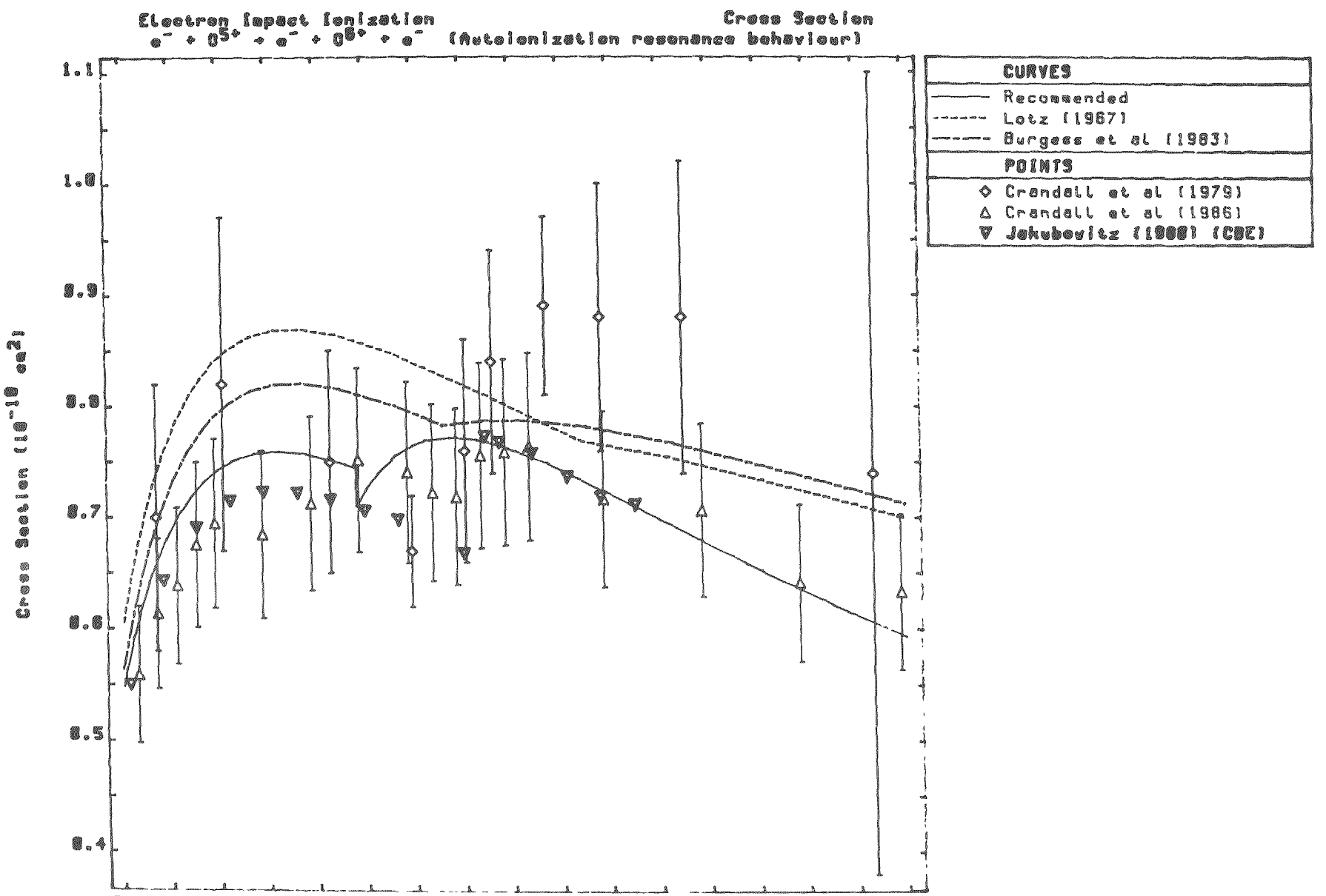
Output Reports

The ouput reports for the example problem are included on the diskette. An example of the output plot from PLOTTAB is illustrated on the next page.


Electron Impact Ionization Cross Section
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1988) (CBE)
Cross Section (10⁻¹⁶ cm²)
1.0
0.8
0.6
0.4
0.2
0.0
10²
10³
10⁴
Incident Electron Energy (eV)


Electron Impact Ionization Cross Section
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻ (Threshold behaviour)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1988) (CBE)
Cross Section (10⁻²¹ cm²)
800
700
600
500
400
300
200
100
0
140
160
180
200
220
240
Incident Electron Energy (eV)


Electron Impact Ionization Cross Section
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻ (Resonance recombination)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1988) (CDE)
Cross Section (10⁻¹⁸ cm²)
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
400
450
500
550
600
650
700
750
800
Incident Electron Energy (eV)


Electron Impact Ionization Cross Section
$e^- + O^{5+} \rightarrow e^- + O^{6+} + e^-$ (Autoionization resonance behaviour)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1988) (CBE)
Cross Section (10^{-18} cm^2)
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Incident Electron Energy (10^3 eV)