INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

IAEA-NDS-219
October 2014
Rev.1 February 2016

IBA-EVAL CHARGED-PARTICLE CROSS-SECTION LIBRARY IN ENDF-6 FORMAT

Andrej Trkov

International Atomic Energy Agency
Vienna, Austria

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

E-mail: NDS.Contact-Point@iaea.org
Fax: (43-1)26007
Telephone: (43-1)2600-21710
Web: http://www-nds.iaea.org

Disclaimer

Neither the author nor anybody else makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information disclosed, or represents that its use would not infringe privately owned rights.

The IAEA-NDS would appreciate any comment on this report at: NDS.Contact-Point@iaea.org.

The IAEA-NDS-reports should not be considered as formal publications. When a nuclear data library is sent out by the IAEA Nuclear Data Section, it will be accompanied by an IAEA-NDS-report which should give the data user all necessary documentation on contents, format and origin of the data library.

IAEA-NDS-reports are updated whenever there is additional information of relevance to the users of the data library.

For citations care should be taken that credit is given to the author of the data library and/or to the data center which issued the data library. The editor of the IAEA-NDS-report is usually not the author of the data library.

Vienna, October 2014

Table of Contents

INTRODUCTION

The Ion-Beam Analysis (IBA) community uses charged-particle interaction data for analytical work. Their interest is usually in the region of relatively low incident energies, where the scattering reactions exhibit pronounced resonance structure, which is utilised for identifying surface and bulk composition of the irradiated materials. They store the data in the so-called R33 Format. On the other hand, most of the existing charged-particle evaluated nuclear data libraries are based on model calculations and do not extend down to low energies, and particularly, they do not include any resonance structure. They are stored in the ENDF-6 Format. The two databases are therefore complementary, but due to the differences in data representation the IBA community has little interaction with other users, and vice-versa. To promote the visibility of the data for both communities it is convenient for the data to be presented in a form that is most commonly used by general users. Nuclear Data Centres archive and disseminate evaluated reaction cross section data in ENDF-6 format and possess software tools for data display and processing. For this reason the ENDF 6 format is well suited as a common basis for the archival of such data.

The Nuclear Data Section (NDS) of the IAEA has supported the activities on nuclear data for IBA and several workshops were organised to train participants in the use of nuclear data for such applications. Some evaluation work was also supported by the IAEA and in fact six evaluations done with the SigmaCalc system of codes were delivered in ENDF-6 Format by the author A. Gurbich; unfortunately the initiative was discontinued. Except for these few, other evaluations are practically "invisible" to the general users outside the IBA community. The policy in the SigmaCalc on-line calculator is to constantly improve and update the database, which is in contradiction with common Quality Assurance (QA) principles and with the policy of NDS to disseminate frozen libraries with strict version control, updated at suitable intervals as deemed necessary. A more extensive set of data from the SigmaCalc system (frozen as of the date of retrieval) is available at the IAEA. The data were downloaded by the program ScGetFromWeb33 (author: V. Zerkin) invoking SigmaCalc 1.6 and SigmaCalc 2.0 (author: A. Gurbich) via the Web interface at the Surrey university Web site in the period from April 2013 to October 2013; during this period the author of SigmaCalc was working under the IAEA Contract NAPC-NDS: PN102725 (22 Oct. 2012 – 23 Oct 2013). The complete set of downloaded files (compressed files in R33 format) is available from the NDS server https://www-nds.iaea.org/public/download-endf/IBA-Eval/SigmaCalcData/. The data were converted into ENDF-6 format at the NDS using the IBAEVAL code (author: A. Trkov) for the benefit of the general users, who might be interested in the low-energy charged particle interaction data.

Note that the conversion into the ENDF-6 format was done without any attempt to optimize data storage. The primary objective was simply to transform the data into a form through which they would be visible and accessible to the users outside the IBA community.

WARNING: The IBA-EVAL library is derived from the SigmaCalc evaluations and is "frozen" as of the date of retrieval. The users who wish to obtain current "state-of-the-art" data for IBA application should go to the IBANDL web page "https://www-nds.iaea.org/exfor/ibandl.htm" and follow the link to the online SigmaCalc retrieval.

SCOPE

In the IBA-EVAL library there are 39 evaluations for reactions with charged particles. The conversion was limited to the elastic scattering reactions, since other reactions require the use of a different format option in ENDF-6. Altogether, 20 reactions were converted into ENDF format. The list of reactions is given in Table 1.

Table 1: List of materials and reactions in the IBA-EVAL library, giving SigmaCalc version and the date of retrieval. Reaction string defines the projectile and the ejectile (p=proton, a=alpha particle); for non-elastic reactions the numerical value after the ejectile refers to the discrete level state.

No.	Target	Reaction	SigmaCalc	Date	ENDF
1	Al-27	(p,p)	1.6.	09-04-2013	Yes
2	Ar-40	(p,p)	1.6.	09-04-2013	Yes
3	C-12	(a,a)	1.6.	08-04-2013	Yes
4	C-12	(d,d)	1.6.	08-04-2013	Yes
5	C-12	(d,p0)	1.6.	08-04-2013	--
6	C-12	(p,p)	1.6.	08-04-2013	Yes
7	C-13	(p,p0)	2.0.	21-06-2013	--
8	Ca-40	(p,p)	1.6.	09-04-2013	Yes
9	Cr-52	(p,p)	1.6.	09-04-2013	Yes
10	Cr-nat	(p,p)	1.6.	09-04-2013	--
11	F-19	(p,p)	1.6.	09-04-2013	Yes
12	Fe-56	(p,p0)	1.6.	06-05-2013	--
13	Fe-nat	(p,p0)	2.0.	27-06-2013	--
14	H-1	(a,p)	2.0.	27-06-2013	--
15	He-4	(p,p0)	2.0.	27-06-2013	--
16	K-39	(p,p)	1.6.	09-04-2013	Yes
17	Mg-24	(a,a)	1.6.	09-04-2013	Yes
18	Mg-24	(p,p)	1.6.	09-04-2013	Yes
19	Mg-nat	(p,p)	1.6.	09-04-2013	--
20	N-14	(a,a)	1.6.	08-04-2013	Yes
21	N-14	(d,a0)	1.6.	03-05-2013	--
22	N-14	(d,a1)	1.6.	03-05-2013	--
23	N-14	(d,p0)	1.6.	08-04-2013	--
24	N-14	(p,p)	1.6.	08-04-2013	Yes
25	Na-23	(p,p)	1.6.	09-04-2013	Yes
26	Ne-20	(p,p)	1.6.	09-04-2013	Yes
27	O-16	(a,a)	1.6.	08-04-2013	Yes
28	O-16	(d,a0)	1.6.	03-05-2013	--
29	O-16	(d,d)	1.6.	08-04-2013	Yes
30	O-16	(d,p0)	2.0.	28-10-2013	--
31	O-16	(d,p1)	2.0.	27-06-2013	--
32	O-16	(p,p)	1.6.	08-04-2013	Yes
33	P-31	(p,p)	1.6.	09-04-2013	Yes
34	S-nat	(p,p)	1.6.	09-04-2013	--

35	Si-28	(p,p0)	2.0.	27-10-2013	--
36	Si-nat	(a,a0)	2.0.	25-10-2013	--
37	Si-nat	(p,p0)	2.0.	27-10-2013	--
38	Ti-48	(p,p)	1.6.	09-04-2013	Yes
39	Ti-nat	(p,p0)	1.6.	09-04-2013	--

DATA PROCESSING AND STORAGE

All files in R33 format at different ejectile angles for every nuclide and reaction were processed with the IBAEND code, specifically written for this purpose. Linear interpolation is assumed between the cosines of the scattering angles, as well as between incident particle energies. Therefore, the data are as accurate as the grid of the angles at which the data files are given, but generally the grid is very dense (usually even excessively dense), hence the interpolation error is considered to be small.

At present, only the elastic scattering data are processed, since these are the most important and rather difficult to handle because of the Coulomb contribution to the scattering, which goes to infinity at forward angles.

The form of data representation in the ENDF-6 format is adapted to the available data. The Coulomb contribution is subtracted from the cross sections. The integral of the remainder over all given angles is stored in the ENDF File-3. The angular distribution of the normalized remainder is stored in File-6 with the flag LTP=12. This form of data representation is fully consistent with ENDF-6 format rules and is also used in many other evaluated nuclear data files; it is processable by the ENDF online retrieval system of the IAEA. The retrieval system restores the Coulomb scattering contribution automatically.

VERIFICATION

Formal correctness of the files in ENDF format was checked with the CHECKR code. It reported that the number of energy points in File-6 was exceeded. This is an administrative format limitation, which does not pose a problem to most processing codes and can be ignored for the time being.

At present, only a limited number of conversion verification tests were performed. For each reaction the cross sections were retrieved from the ENDF file at 60 degrees and at 160 degrees and compared directly to the original data in R33 format. The procedure confirmed the accuracy of the transformation. An example of a satisfactory verification plot is shown in Figure 1. In some cases insufficient precision (limited to 5 digits) was found in the printed energy in the R33 output from SigmaCalc. Consequently, the data for ^{52}Cr(p,p) contain several duplicate energy points, and in some cases the energy grid is not monotonic. An example of the diagnostic printout is given below:

```
WARNING - Non-monotonic energy grid 3.21780E+06 3.21810E+06 3.21810E+06
WARNING - Non-monotonic energy grid 3.23840E+06 3.23880E+06 3.23880E+06
WARNING - Non-monotonic energy grid 3.32000E+06 3.32050E+06 3.32050E+06
WARNING - Non-monotonic energy grid 3.39050E+06 3.39100E+06 3.39100E+06
WARNING - Non-monotonic energy grid 3.44910E+06 3.45000E+06 3.44940E+06
WARNING - Non-monotonic energy grid 3.45920E+06 3.45950E+06 3.45940E+06
WARNING - Non-monotonic energy grid 3.47800E+06 3.47860E+06 3.47840E+06
WARNING - Non-monotonic energy grid 3.48150E+06 3.48210E+06 3.48180E+06
WARNING - Non-monotonic energy grid 3.48850E+06 3.48890E+06 3.48890E+06
WARNING - Non-monotonic energy grid 3.51800E+06 3.51870E+06 3.51840E+06
WARNING - Non-monotonic energy grid 3.56740E+06 3.56790E+06 3.56780E+06
WARNING - Non-monotonic energy grid 3.57300E+06 3.57360E+06 3.57310E+06
WARNING - Non-monotonic energy grid 3.60540E+06 3.60570E+06 3.60570E+06
WARNING - Non-monotonic energy grid 3.63840E+06 3.63910E+06 3.63870E+06
WARNING - Non-monotonic energy grid 3.63910E+06 3.63870E+06 3.63860E+06
WARNING - Non-monotonic energy grid 3.64830E+06 3.64890E+06 3.64890E+06
WARNING - Non-monotonic energy grid 3.65120E+06 3.65170E+06 3.65140E+06
WARNING - Non-monotonic energy grid 3.67900E+06 3.67920E+06 3.67920E+06
WARNING - Non-monotonic energy grid 3.68630E+06 3.68680E+06 3.68670E+06
WARNING - Non-monotonic energy grid 3.69390E+06 3.69410E+06 3.69410E+06
WARNING - Non-monotonic energy grid 3.69860E+06 3.69880E+06 3.69880E+06
WARNING - Non-monotonic energy grid 3.72840E+06 3.72880E+06 3.72880E+06
WARNING - Non-monotonic energy grid 3.74680E+06 3.74710E+06 3.74670E+06
WARNING - Non-monotonic energy grid 3.84090E+06 3.84130E+06 3.84130E+06
WARNING - Non-monotonic energy grid 3.87090E+06 3.87120E+06 3.87120E+06
WARNING - Non-monotonic energy grid 3.87570E+06 3.87610E+06 3.87610E+06
WARNING - Non-monotonic energy grid 3.91110E+06 3.91150E+06 3.91140E+06
WARNING - Non-monotonic energy grid 3.95490E+06 3.95550E+06 3.95500E+06
WARNING - Non-monotonic energy grid 3.97670E+06 3.97700E+06 3.97690E+06
WARNING - Non-monotonic energy grid 4.02150E+06 4.02160E+06 4.02160E+06
WARNING - Non-monotonic energy grid 4.06380E+06 4.06420E+06 4.06410E+06
WARNING - Non-monotonic energy grid 4.06880E+06 4.06910E+06 4.06910E+06
WARNING - Non-monotonic energy grid 4.07040E+06 4.07070E+06 4.07070E+06
WARNING - Non-monotonic energy grid 4.07470E+06 4.07520E+06 4.07520E+06
WARNING - Non-monotonic energy grid 4.07990E+06 4.08000E+06 4.07990E+06
WARNING - Non-monotonic energy grid 4.08000E+06 4.07990E+06 4.07990E+06
WARNING - Non-monotonic energy grid 4.08580E+06 4.08590E+06 4.08590E+06
WARNING - Non-monotonic energy grid 4.15010E+06 4.17504E+06 4.15030E+06
WARNING - Non-monotonic energy grid 4.17600E+06 4.17660E+06 4.17660E+06
WARNING - Non-monotonic energy grid 4.17830E+06 4.17860E+06 4.17860E+06
```

The out-of-sequence energy was set to the mid-point of its neighbours to make the ENDF file formally correct, although this is an ad-hoc action, which should be resolved in the original evaluation.

Additional verification was performed by plotting angular distributions at three energies, spaced at 1/4, 1/2 and 3/4 of the energy range. The distributions passed the test for continuity of the distribution.

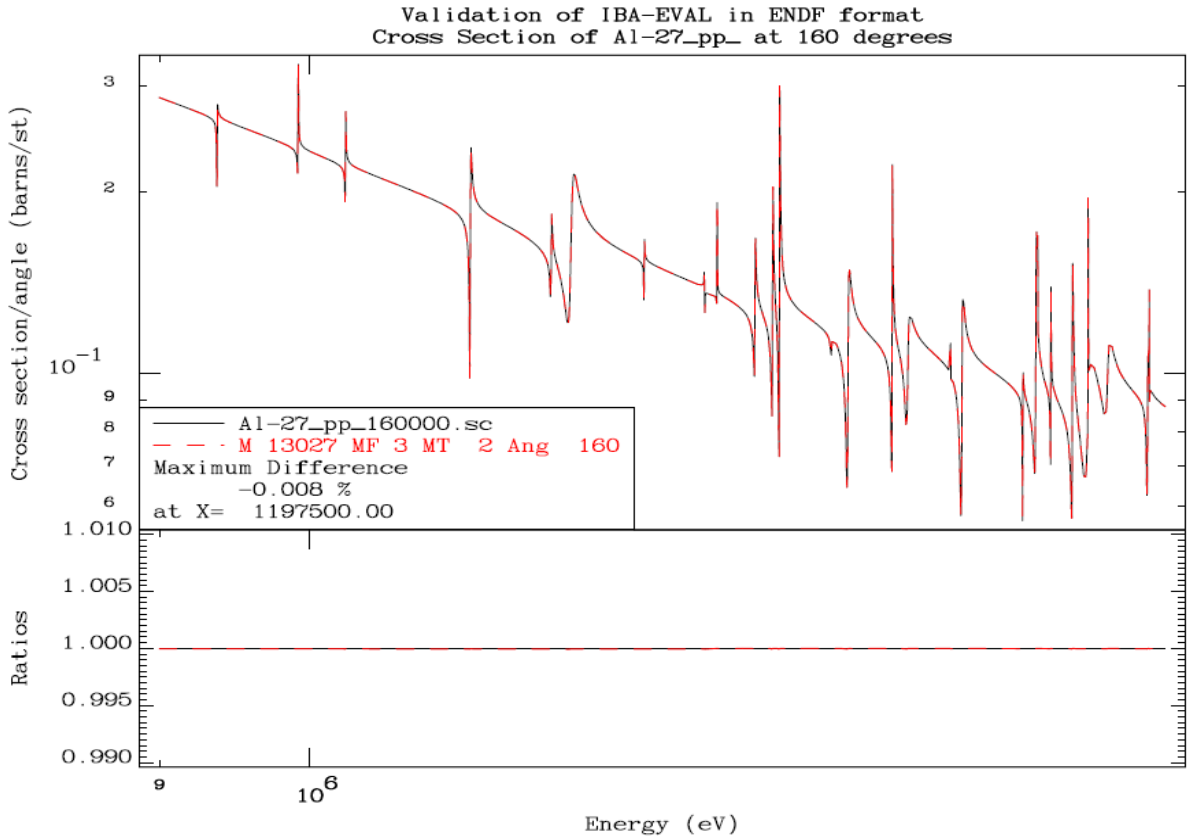

Figure 1: Example of a verification plot, comparing the data from R33 file with that retrieved from the ENDF file at 160 degrees.

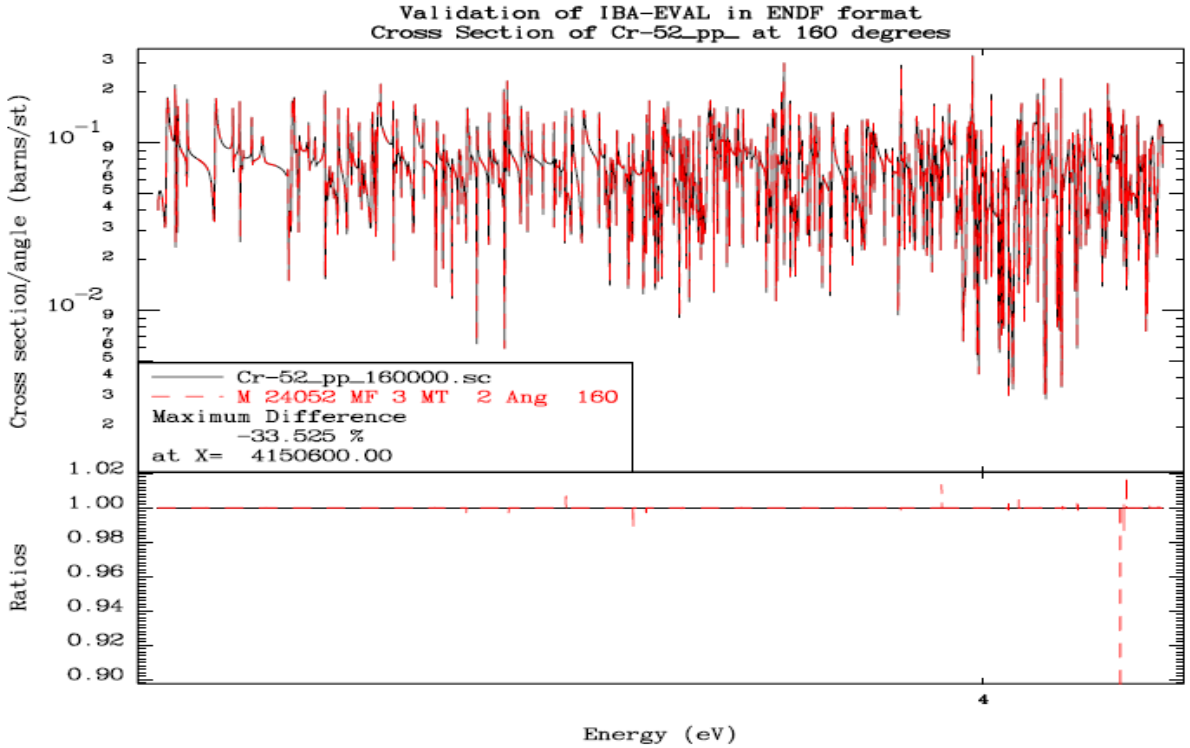

Figure 2: Example of a verification plot showing differences, caused mainly by the insufficient precision of the printed energy in the R33 file and a single case of non-monotonic energy grid.