IAEA-TECDOC-Draft

Reference Input Parameter Library

Handbook for calculations of nuclear reaction data

Final report of a co-ordinated research project

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FOREWORD

Nuclear data for applications constitute an integral part of the IAEA programme of activities. When considering low-energy nuclear reactions induced with light particles, such as neutrons, protons, deuterons, alphas and photons, one addresses a broad range of applications, from nuclear power reactors and shielding design through cyclotron production of medical radioisotopes and radiotherapy to transmutation of nuclear waste. In all these and many other applications one needs a detailed knowledge of cross sections, spectra of emitted particles and their angular distributions and of isotope production.

A long-standing problem — how to meet nuclear data needs of the future with limited experimental resources — puts a considerable demand upon nuclear model computation capabilities. Originally almost all nuclear data was provided by measurement programs. Over time, theoretical understanding of nuclear phenomena has reached a considerable degree of reliability, and nuclear modeling has become an important source of evaluated nuclear data (with measurements remaining critical for data testing and benchmarking).

The practical use of nuclear model codes requires a considerable numerical input that describes properties of the nuclei and interactions involved. Leading nuclear data laboratories and experts have used a variety of different input sets, often developed over years in their own laboratories. Many of these partial input databases were poorly documented, or not documented at all, and not always available for other users. With the trend of reduced funds for nuclear data evaluations, there is a real threat that the accumulated immense knowledge on input parameters and the related state-of-the-art may be reduced or even lost for the future applications.

Given this situation, a project was proposed, with the aim to develop an internationally recognized input parameter library, with contributions from all major players around the world. The idea was discussed in the nuclear data community in the beginning of 1990s and it was enthusiastically supported by the International Nuclear Data Committee as a top priority nuclear data project for the IAEA.

An ultimate objective of any international effort along these lines is to develop a library of evaluated and tested nuclear-model input parameters. Considering that such a task indeed is immense, it was decided to proceed in two major steps. First, to summarize the present knowledge on input parameters, and whenever possible to critically analyze these paramaters and to develop a single Starter File of input model parameters. This data base will be of immediate practical value for a number of users and should represent a firm basis for any future improvements and developments. The second step will focus on the testing, validation and related improvement of the Starter File.

With these objective in mind the IAEA initiated a Coordinated Research Project (CRP) under the title *"Development of Reference Input Parameter Library for Nuclear Model Calculations of Nuclear Data (Phase I: Starter File)"*. The project, coordinated by the IAEA between 1994 and 1997, produced two major results. First, the complete electronic Starter File was developed and made available to users cost-free throughout the world. Second, the present Handbook was prepared, containing a detailed description of the library.

The IAEA wishes to thank all the participants of the CRP, and also other scientists associated with the project, for their diligent work that lead to the creation of the Reference Input Parameter Library and for their most valuable contributions to the present TECDOC.

SUMMARY

The Reference Input Parameter Library (RIPL) contains input parameters for theoretical calculations of nuclear reaction cross sections. The library is targeted at users of nuclear reaction codes interested in low-energy nuclear applications. Incident and outgoing particles include n, p, d, t, ^{3}He, ^{4}He and γ, with the energies up to about 100 MeV.

RIPL is being developed under an international project coordinated by the IAEA. Phase I of the project, conducted in 1994-1997, resulted in the creation of the RIPL Starter File (numerical data) and the present RIPL Handbook.

RIPL Starter File. The Starter File contains numerical data arranged in seven segments/directories:

```
No  Directory    Contents
..  ...........  .......................................
1   MASSES       Atomic Masses and Deformations
2   LEVELS       Discrete Level Schemes
3   RESONANCES   Average Neutron Resonance Parameters
4   OPTICAL      Optical Model Parameters
5   DENSITIES    Level Densities (Total, Fission, Partial)
6   GAMMA        Gamma-Ray Strength Functions
7   ANGULAR      Continuum Angular Distributions
```

Each segment/directory is split into two subdirectories:

- RECOMMENDED (for recommended input parameters), and
- OTHER_FILES (for alternative input parameters and other useful data).

The Starter File, physically located at the DEC Alpha server operated by the IAEA Nuclear Data Section, can be conveniently accessed using the Web interface or by using FTP. The address of the Web site reads

```
http://www-nds.iaea.or.at/ripl/
```

while for FTP one should use

```
ftp iaeand.iaea.org
username: ripl
```

with no password required. In addition, complete Starter File on a CD-ROM is available from the IAEA Nuclear Data Section cost-free upon request.

RIPL Handbook. The Handbook contains description of the library, including the physics involved. It consists of Introduction, seven Chapters and three Appendices. The chapters follow the structure explained above, the Appendices include the list of files in the Starter File and reproduce two important papers devoted to the optical model.

Contents

Introduction

An important trend in the evaluation of neutron and charged-particle nuclear data at low energies (0-30 MeV) is the increased use of nuclear reaction theory codes to compute the cross sections, spectra, and angular distributions required by a large variety of applications. As a method of evaluation, such model codes offer, in comparison with simpler approaches, many advantages such as the preservation of the energy balance or the coherence of partial cross sections with the total or the reaction cross section, which are essential properties for nuclear data used in transport calculations. In addition, the theoretical approach is the only one that allows to predict data for unstable nuclei.

For any nuclear reaction calculation nuclear masses are very basic data for getting binding energies or Q-values. They are presented in **Chapter 1** together with other useful information such as ground state deformations.

Discrete level schemes, including spins, parities, γ-transitions and branching are important for establishing of low-energy nuclear level densities and for related cross section calculations. Most of the corresponding experimental information are contained in the ENSDF library and **Chapter 2** describes the procedures used to retrieve the needed data.

As is well known, the neutron cross sections at low incident energies present a resonant behaviour, and a careful statistical analysis of the experimental results leads to the average neutron resonance parameters, as described in **Chapter 3**. These average quantities are not directly used in the model calculations but are important data for constraining the parameters of different models:

- the average spacing of resonances is the only measure of the level density near the neutron binding energy,
- the neutron strength functions have to be reproduced by the optical model at low energy, and
- the average radiative width is used as a normalization for the gamma-ray strength functions.

Above the resonance energy region, the nuclear reaction models only reproduce the smooth behavior of the cross sections, and the evaluation of nuclear data is generally divided into two major steps.

By using the optical model in the first step, the elastic channel and the direct inelastic ones for deformed nuclei are explicitly calculated whereas all other channels are lumped together in the reaction cross section. **Chapter 4** gives an extensive compilation optical model parameter sets for different types of incident particles, from neutron to ^{4}He. In order to produce a consistent evaluation, it is recommended to use, for each interacting system, a unique parameterization which reproduces the relevant observables (total or reaction cross sections, elastic angular distributions, analysing powers) over an energy range as broad as possible, including, in the case of neutron interaction, the low energy region where the calculated neutron strength function and scattering radius should match the experimental values. Furthermore, the parameters should have a smooth energy dependence.

The second step consists in sharing the reaction cross section among all the possible individual channels, as illustrated by Figure 0.1. For incident energies lower than around 10 MeV, this is done by using the statistical decay of the compound nucleus, a formalism often referred to as the Hauser-Feshbach theory. Written in a compact form, the Hauser-Feshbach formula giving

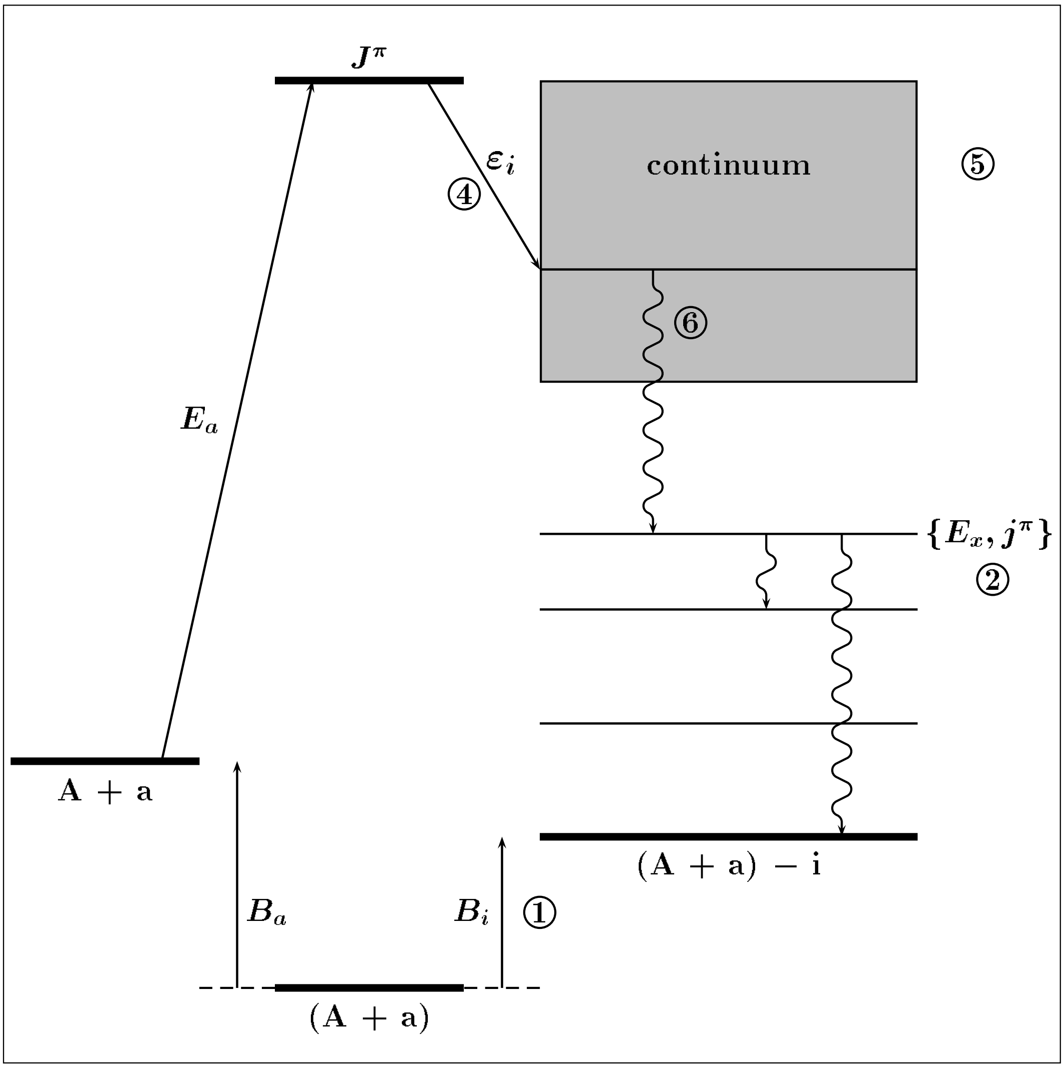

Figure 0.1: Schematic energy diagram of a nuclear reaction. Circled numbers refer to chapters where the parameters are described.

the cross section for the A(a,b)B reaction reads

$$\sigma_{a \to b} = \sum_{J^\pi} \frac{T_a \, T_b}{\sum_i \sum_c T_{ic}}$$

where the index i stands for the different types of outgoing particles[1] (or the fission channel, if any), and the T's are the transmission coefficients calculated by the optical model for this particle. The index c represents all the accessible final states which are either discrete excited levels of the residual nucleus or a continuum of levels described by a level density.

In the case of discrete levels one should only take into account the low-lying levels of known excitation energy, spin, parity, and decay branchings (if γ-production is needed).

Above the energy of the last level for which one of the previous quantities is missing or uncertain, one has to consider a continuum of levels described by a total level density which, at low excitation energy, must match the cumulative number of discrete levels, and, at the neutron binding energy, must reproduce the average spacing of resonances. **Chapter 5.1** presents different theoretical approaches of this longstanding problem.

[1]Generally, the considered outgoing particles are p, n, d, t, ^{3}He, α, and γ.

The fission cross section calculation strongly depend on two key ingredients:

- the fission level density (the level density of the fissioning nucleus at the saddle point deformation), and
- the fission barrier.

These two strongly interdependent parameters are described in **Chapter 5.2**.

For incident energies higher than about 10 MeV, the pre-equilibrium reaction mechanism constitutes the bridge between fast, direct processes and slow compound processes and provides an explanation for the high-energy tails in spectra and the smoothly forward peaked angular distributions. Methods for calculating partial (or particle-hole) level densities for use in pre-equilibrium model calculations are given in **Chapter 5.3**.

Gamma-ray emission channel is an almost universal reaction channel since gamma rays, in general, accompany the emission of any other emitted particle. Here, the basic quantity is the gamma-ray strength function which is discussed in **Chapter 6**.

Besides sophisticated quantum-mechanical models of pre-equilibrium reactions such as the one by Feshbach, Kerman and Koonin, the Kalbach systematics formula to describe the continuum angular distributions of emitted particles represents for most applications an invaluable tool due to its wide-ranging applicability; it is described in **Chapter 7**.

Finally, it should be reminded that many of the parameters needed in the calculations are model dependent and should therefore be used within the strict frame of their definitions.

All the parameters reported in this Handbook can already be used but some of them still need improvements, in particular the optical model part in the light of new developments, and the total level densities which have to reproduce in a consistent way different pieces of information.

The main **Chapters** are followed by three **Appendices**. **Appendix I** brings the basic information on the **recommended files**, which are printed using **bold** font throughout this Handbook as well as on *other* RIPL files (their names are given in *italics*), the directory structure and the file access.

Appendices II and **III** summarize experiences with use of the optical model and its parameters at Los Alamos, where systematics study of this topic has been performed over years.