CM2Lab User's Guide

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1 Introduction

CM2Lab is a program for the conversion of cross-section data from the center-of-mass (CM) to the laboratory system. CM2Lab can be used for

1. elastic scattering cross sections,
2. nuclear reactions cross sections.

Many cross section data for elastic scattering and nuclear reactions were measured in the fifties and sixties and were published in the center-of-mass system. If these cross-section data are intended to be used for simulation calculations with SIMNRA, they have to be converted to the laboratory system. This can be done with the program CM2Lab.

1.1 Conventions in this manual

This manual uses the following conventions:

- Links to sections, figures, tables, or pages are highlighted in red. A click with the mouse will bring you to the link destination.
- Links to references are highlighted in green. A click with the mouse will bring you to the reference.
- Links to internet web sites are highlighted in blue. A click with the mouse will start your web-browser and open the web page.
- Links to other PDF documents are highlighted in cyan. A click with the mouse will open the document.

2 Installation

The files `CM2Lab.exe` and `CM2Lab_Manual.pdf` must be installed in the SIMNRA base directory, i.e. in the directory where `SIMNRA.exe` is located.

3 Using CM2Lab

CM2Lab is a console application without graphical user interface. To use CM2Lab, you have to

1. create a R33 file with the cross-section data in the center-of-mass system. See the section about the R33 file format in the SIMNRA User's Guide for a description of the R33 file format. The full R33 specification can be found in the Appendix of the SIMNRA User's Guide. See section 3.1 for details, which information is required by CM2Lab, and if this information has to be in the center-of-mass or laboratory system.
2. Run CM2Lab, either
   a) By drag and drop of the R33 file onto the CM2Lab symbol. You can drag and drop more than one file.
   b) By opening a command shell (DOS window) and typing `CM2Lab FileName.R33`, where `FileName.R33` is your R33 file. If the file is located in a different directory, the full path to the file has to be specified. If the file name contains blanks, it has to be surrounded by " (`"FileName.R33"`). You can specify more than one file. File names are separated by blanks.
3. CM2Lab creates two files:
   a) `FileName.Lab.R33` is in R33 format and contains the cross-section data in the laboratory system.
   b) `FileName.out` contains additional information (masses, CM energy, CM angle, etc.) about the calculation. This file can be used for diagnostic purposes.

3.1 The R33 input file

The R33 file with cross-section data in the center-of-mass system must contain at least the following information:

- A line containing the string 'Reaction:'. The nuclear reaction string (for example 16O(d,a0)14N) written in that line is interpreted to find out which particles are involved in the reaction. The masses of the particles are ignored.

- A line containing the string 'Masses:'. The masses of the particles are taken from this line. All masses in amu. The first mass is the mass of the incident particle, the second mass is the mass of the target particle, the third mass is the mass of the outgoing particle for which the cross-section is valid, and the fourth mass is the mass of the other reaction product. The masses may be rounded to the nearest integer value - they are replaced by the precise values.

  Warning: Note that the masses are given in a different order than in the 'Reaction' string! For the reaction 16O(d,a0)14N the correct line is 'Masses: 2, 16, 4, 14'. This is a permanent source of error, so check your input carefully.

- A line containing the string 'QValue:'. The Q-value is the energy released in the nuclear reaction (in keV). Q = 0.0 for elastic scattering.

- A line containing either the string 'Theta:' or 'Theta_CM:'. Theta is the scattering or reaction angle *in the laboratory system*, while Theta_CM is the angle *in the center-of-mass system*. Theta or Theta_CM are in degrees. If Theta_CM is given, then CMToLab will replace the center-of-mass angle by the corresponding angle in the laboratory system.

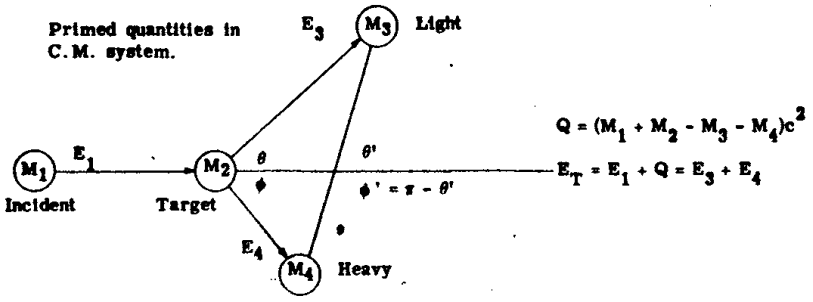
- A line containing the string 'Data:'. The cross-section data have to start after this line. The cross-section data are *in the center-of-mass system*.

- The data are organized in 4 columns: The first column is the *laboratory energy* of the incident particle in keV, the second column is the energy error in keV), the third column is the differential cross-section *in the center-of-mass system*, and the fourth column is the cross-section error *in the center-of-mass system*. The cross section must be in mbarn/sr. The cross-section and the cross-section error are converted to the laboratory system. The data should be arranged in order of ascending energy.

An example of a valid R33 cross-section data file can be found in the SIMNRA User's Guide.

4 Physics

The used quantities and the relations between them are shown in Figure 4.1. See also [1, Appendix 4].



Define:

$$A_{14} = \frac{M_1 M_4 (E_1/E_T)}{(M_1 + M_2)(M_3 + M_4)}, \qquad A_{23} = \frac{M_2 M_3}{(M_1 + M_2)(M_3 + M_4)} \left(1 + \frac{M_1}{M_2}\frac{Q}{E_T}\right) = \frac{E_4'}{E_T}$$

$$A_{13} = \frac{M_1 M_3 (E_1/E_T)}{(M_1 + M_2)(M_3 + M_4)}, \qquad A_{24} = \frac{M_2 M_4}{(M_1 + M_2)(M_3 + M_4)} \left(1 + \frac{M_1}{M_2}\frac{Q}{E_T}\right) = \frac{E_3'}{E_T}$$

Note that $A_{14} + A_{13} + A_{23} + A_{24} = 1$

Lab energy of light product:	$\frac{E_3}{E_T} = A_{13} + A_{24} + 2(A_{14}A_{23})^{\frac{1}{2}} \cos\theta' = A_{13}\left[\cos\theta \pm (A_{24}/A_{13} - \sin^2\theta)^{\frac{1}{2}}\right]^2$	Use only plus sign unless $A_{13} > A_{24}$, in which case $\theta_{max} = \sin^{-1}(A_{24}/A_{13})^{\frac{1}{2}}$
Lab energy of heavy product:	$\frac{E_4}{E_T} = A_{14} + A_{23} + 2(A_{14}A_{23})^{\frac{1}{2}} \cos\phi' = A_{14}\left[\cos\phi \pm (A_{23}/A_{14} - \sin^2\phi)^{\frac{1}{2}}\right]^2$	Use only plus sign unless $A_{14} > A_{23}$, in which case $\phi_{max} = \sin^{-1}(A_{23}/A_{14})^{\frac{1}{2}}$
Lab angle of heavy product:	$\sin\phi = \left(\frac{M_3 E_3}{M_4 E_4}\right)^{\frac{1}{2}} \sin\theta$	**C.M. angle of light product:** $\sin\theta' = \left(\frac{E_3/E_T}{A_{24}}\right)^{\frac{1}{2}} \sin\theta$
Intensity or solid-angle ratio for light product:	$\frac{\sigma(\theta')}{\sigma(\theta)} = \frac{I(\theta')}{I(\theta)} = \frac{\sin\theta\, d\theta}{\sin\theta'\, d\theta'} = \frac{\sin^2\theta}{\sin^2\theta'} \cos(\theta' - \theta) = \frac{(A_{14}A_{23})^{\frac{1}{2}} (A_{24}/A_{13} - \sin^2\theta)^{\frac{1}{2}}}{E_3/E_T}$	
Intensity or solid-angle ratio for heavy product:	$\frac{\sigma(\phi')}{\sigma(\phi)} = \frac{I(\phi')}{I(\phi)} = \frac{\sin\phi\, d\phi}{\sin\phi'\, d\phi'} = \frac{\sin^2\phi}{\sin^2\phi'} \cos(\phi' - \phi) = \frac{(A_{14}A_{23})^{\frac{1}{2}} (A_{23}/A_{14} - \sin^2\phi)^{\frac{1}{2}}}{E_4/E_T}$	
Intensity or solid-angle ratio for associated particles in the lab system:	$\frac{\sigma(\phi)}{\sigma(\theta)} = \frac{I(\phi)}{I(\theta)} = \frac{\sin\theta\, d\theta}{\sin\phi\, d\phi} = \frac{\sin^2\theta}{\sin^2\phi} \frac{\cos(\theta' - \theta)}{\cos(\phi' - \phi)}$	

Figure 4.1: Quantities used for the calculation of nuclear reaction kinematics. From [2].

5 Version history

Version 1.1

Changes

1. Cross-section error bars are converted from the center-of-mass to the laboratory system as well.

2. The scattering angle may be given in the center-of-mass system.

Bibliography

[1] J.R. Tesmer and M. Nastasi, Eds. *Handbook of Modern Ion Beam Materials Analysis*. Materials Research Society, Pittsburgh, Pennsylvania, 1995. 5

[2] N. Jarmie and J.D. Seagrave. Charged particle cross sections. Tech. Rep. LA-2014, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico, U.S.A., 1956. 6