

X.A. ANGODF: CONVERT FROM ENERGY/ANGLE TO ANGLE/ENERGY

When analyzing angular distribution data (differential elastic scattering), the results are reported in two ODF files. The first file, SAMMY.DAT, contains the experimental data and uncertainties for each angle, as a function of energy; contents of each section of this file are shown in Table X A.1. The second file, SAMMY.ODF, contains the results of the calculations; contents of this file are described in Table X A.2. Note that the angles themselves are not listed in these files; they are only in the user's INPut file, card set 8.

Table X A.1. Contents of the ODF file SAMMY.DAT

Sect. No.	Meaning
1	Energy in eV
2	Experimental cross section (barns) for the first angle
3	Absolute uncertainty on experimental cross section for the first angle
4	Experimental cross section (barns) for the second angle
5	Absolute uncertainty on cross section (barns) for the second angle
6,7, etc.	Repeat, two sections (data plus uncertainty) for each angle

Table X A.2. Contents of the ODF file SAMMY.ODF for angular distribution data

Sect. No.	Meaning
1	Energy in eV
2	Initial calculation of cross section (barns) for the first angle
3	Final calculation of cross section (barns) for the first angle
4	Initial calculation of cross section (barns) for the second angle
5	Final calculation of cross section (barns) for the second angle
6,7, etc.	Repeat, two sections (initial plus final calculation) for each angle

Using these two files, one can produce plots of the various cross sections (experimental vs calculated) at a given angle, with energy as the horizontal axis. Often, however, it is also useful to consider plots of cross sections at a given energy, with angle as the horizontal axis, which cannot be accomplished directly with forodf. Instead, the positions of energy and angle must be reversed in a new ODF file; this can be accomplished using the conversion program ANGODF.

To run program ANGODF, respond appropriately to the following questions:

- What is name of ODF file with experimental data? [SAMMY.DAT]
- What is name of ODF file with theoretical values? [SAMMY.ODF]
- What is name of new ODF file? [whatever name you choose]
- What is name of INPut file? [same as the INPut file that was used to generate SAMMY.DAT and SAMMY.ODF]
- Are all energies to be used? (default = NO)
- What energies? One per line, end with blank... [question is omitted if response to previous question was "yes"]

The program will generate an ODF file (with the name you chose), containing sections as described in Table X A.3.

Table X A.3. Contents of the ODF file created by program ANGODF

Sect. No.	Meaning
1	Angle in degrees
2	Experimental cross section (barns) for the first energy
3	Absolute uncertainty on the experimental cross section (barns)
4	Initial calculation of cross section (barns) for the first energy
5	Final calculation of cross section (barns) for the first energy
6,7, etc.	Repeat, four sections (data plus uncertainty, initial plus final calculation) for each energy requested