VI.C.1. Experimental Data

The original format for the DATa file is shown in Table VI C1.1; this version is borrowed directly from MULTI [GA74]. Three data points, including energy, experimental value for cross section (or transmission, eta, etc.), and relative uncertainty appear on each line. Energies may be ordered from high to low or low to high, but the ordering must be monotonic. The data file may contain points that are not within the range [EMIN,EMAX] specified for this run; such points will be ignored (or, possibly, used for determining the auxiliary grid. See Section III.A).

A second ASCII format permits one data point per line, in (3F11) or (3E11) format, with uncertainties being absolute (rather than relative as in the "original" format). To use this option, the phrase "`USE CSISRS FORMAT FOr data`" or an equivalent must appear in card set 3 of the INPut file (See Table VI A1.2).

A third ASCII format is useful when many significant digits are needed (e.g., when comparing cross sections calculated by SAMMY with those calculated by other codes). This format has one data point per line, in (3F20) or (3E20) format, and uncertainties are absolute. The phrase "`USE TWENTY SIGNIFICAnt digits for experimental data`" (or simply "`TWENTY`") must appear in card set 3 of the INPut file (Table VI A1.2).

The energies and cross sections from an ENDF/B File 3 listing may be used for the "experimental data" in a SAMMY run. The command for this option is "`USE ENDF/B ENERGIES and cross sections MAT=`abcd", in which "abcd" is replaced by the ENDF MAT (material) number. See test case tr086 for examples.

For ORNL-ORELA staff and others who use the plotting package FORODF [JC78] with their version of SAMMY, there are several possible methods of supplying data in ORELA Data Format (ODF): For the first, you must specify "`DATA ARE IN ODF FILE`" in card set 3 of the INPut file (see Tables VI A.1 and VI A1.2). In this ODF data file, section 1 contains the energy (which can be either high-to-low or low-to-high), section 2 contains the data, and 3 contains the absolute uncertainty. Use of this alternative is discouraged, because SAMMY handles it awkwardly, copying to a temporary file in the usual DATa file format of Table VI C1.1. See test case tr005 for an example using this option.

The second ODF format is the "standard ODF format," for which you must specify "`DATA ARE IN STANDARD odf format`" in your input file. In this ODF file, unlike the version in the previous paragraph, the energies must be ordered high to low. Again energies are stored in section 1, data in section 2, and absolute uncertainties in section 3. The standard ODF file contains additional sections not in the other version: sections 4, 5, and so forth are used to store the partial derivatives of the data with respect to the data-reduction parameters. (See Section III.E.3 of this report for a discussion of data-reduction parameters.) Note that section 4 of the ODF file must correspond to data-reduction parameter number 1, section 5 to parameter number 2, etc. As with all varied parameters, initial values are given in the PARameter file (card set 8 of Table VI B.2). This method has not been used very much and will likely be dropped in future releases.

Two options are available for specifying differential elastic scattering data. The first is via an ODF file. Section 1 of this file contains the energy; section 2, the measured cross sections for the first angle; section 3, the absolute uncertainties on the cross sections in section 2; sections 4 and 5, the cross sections and uncertainties for the second angle; and so forth. In general, section $2n$ contains data for the n^{th} angle; and section $2n+1$ contains the uncertainties. Angles are specified in the INPut file, card set 8 (see Table VI A.1). (This option has seen little use and will likely be dropped in future revisions.)

The second option for differential elastic data is via an ASCII file, all in (8F10.1) format, with at least two lines per energy. The first line contains the energy in the first ten columns, cross section at first angle in columns 11-20, cross section at second angle in columns 21-30, etc.; if there are more than seven angles, the eighth appears in columns 1-10 of the next line. The second line (or set of lines) is blank in columns 1-10, contains the (absolute) uncertainty in the cross section at the first angle in columns 11-20, uncertainty for the second angle in columns 11-20, etc.; again, if there are more than seven angles, then values for the 8^{th} and subsequent angles are on additional lines, beginning in column 1. These two (sets of) lines are repeated once for each energy. To use this option, it is necessary to include the phrase "`DIFFERENTIAL DATA ARE IN ascii file`" in the INPut file. See test cases tr033, tr043, tr109, and others for examples.

Table VI C 1.1. MULTI-Style Format for the DATa file

Line	Column	Variable	Format	Meaning (units)
1,2,etc.	1-15	$ENERGY_1$	F15	Energy (eV)
	16-30	$DATA_1$	F15	Experimental cross section (barns), transmission, yield, or other type of data
	31-37	$FRACT_1$	F7	Fractional uncertainty in $DATA_1$
	38-52	$ENERGY_2$	F15	
	53-67	$DATA_2$	F15	
	68-74	$FRACT_2$	F7	
	75-89	$ENERGY_3$	F15	
	90-104	$DATA_3$	F15	
	105-111	$FRACT_3$	F7	

Note that although F formats are specified above, input can be in either E or F format. Numbers must, however, be within the columns specified, and a decimal point is required. If using E format, the exponent is in the right-most columns.