

Finally, a single input command will alter the ordering of the spin groups from $\{J, \pi\}$ as in the 2003 version to $\{L, J\}$ (where L here indicates the orbital angular momentum of the first entrance channel for any given spin group, and J and π indicate the total angular momentum and parity for the spin group).

Table X J.1 summarizes the input options for the particle-pair mode.

Test case tr143 gives numerous examples of the use of this code. Cases whose names end in “a” use the Cadarache mode of SAMQUA input, and cases whose names end in “b” use the particle-pair mode. Cases labeled with “c” include the option to read channel radii from a separate file, and cases labeled with “d” provide reordered output. Cases labeled “e” read from a parameter file to learn energies on which to calculate penetrabilities and hard-sphere cross sections.

Table X J.1. Input options for SAMQUA in particle-pair mode

Line	Contents	Notes	Required?
1	Title	1. Alphanumeric title, will be printed but not used.	Yes
2,3, ...	Blank, or containing # in first column.	1. Blank or # lines may be inserted almost anywhere into the file.	No
4, 5	“EMIN =” <i>or</i> “EMAX =”, followed by the real value.	1. The penetrability and hard-sphere cross section will be calculated at Emin, (Emin+Emax)/2, and Emax. 2. If either Emin or Emax is unspecified, the default values (1 eV, 1 MeV respectively) will be used. 3. The equal sign <i>must</i> be included.	No
Alt. 4 (no 5)	“ENERgy file =”, followed by name of file in which energies are stored	1. Energies are listed one per line, in the first eleven columns. 2. A SAMMY-style resonance PARAmeter file can be used here (in which case negative energies and continuation lines will be ignored).	No
6	“RADIus file =”, followed by the name of the file in which the radii are stored	1. The “radius file” defines values for the channel radii, which are needed for calculating the penetrabilities and hard-sphere cross sections. The format for the radius file is the same as card set 7a of the PARAmeter file, with the caveat that only particle-pair and orbital angular momentum information can be given, and not spin group and channels (since these will be determined by the samqua run).	No

Table X J.1 (continued)

Line	Contents	Notes	Required?
6, cont.		<ol style="list-style-type: none"> 2. If channel radii are not specified (i.e., if this line is absent and no “radius file” exists), the SAMQUA default values are used. 3. Only the first three characters of “radius file” are needed; however, the equal sign <i>must</i> be included. 4. This line may be interchanged with line 7. 	
7	“REOrder according to LJ not Jpi” or “ORDer by LJ”.	<ol style="list-style-type: none"> 1. If this line is present, the spin groups will be listed in the output files in order of increasing L, where L here refers to the orbital angular momentum of the first (incident) channel for each spin group. If two spin groups have the same value of L, the one with the smaller value of J will be listed first. 2. If this line is absent, the spin groups are ordered by increasing J, with negative-parity spin groups listed before those with positive parity. 3. This line may be interchanged with line 6. 	No
8	“NUclide, Lmax=” or “First nuclide, Lmax=”, followed by integer value for Lmax. Line may also contain “Number of fission channels =”, followed by integer value	<ol style="list-style-type: none"> 1. Indicates the beginning of information for the first nuclide. Only the first two characters (NU) and the first equal sign are required. 2. Lmax is the maximum value of the orbital angular momentum. 3. If a second equal sign is present, the integer value following that equal sign is the number of fission channels to be included. 	Yes
9	“Abundance =”, followed by real value	<ol style="list-style-type: none"> 1. Indicates the abundance of this isotope. Printed in file quanpar.dat for use in card set 10 of the SAMMY PARAmeter file. 2. No blank line (or # line) is permitted between Line 8 and Line 9. 	Yes
10, etc.		<ol style="list-style-type: none"> 1. These lines give the particle-pair information, exactly as in card set 4 of the INPut file. 2. End with a blank line (<i>not</i> a # line) 	Yes

Table X J.1 (continued)

Line	Contents	Notes	Required?
11	<p>“NUCLide, Lmax=” or “NEXT nuclide, Lmax=” or “NEW nuclide, Lmax=”</p> <p>Line may also contain “Number of fission channels =”, followed by integer value</p>	<p>Like line 8 for another nuclide:</p> <ol style="list-style-type: none"> 1. Indicates the beginning of information for the new nuclide. Only the first four characters and the first equal sign (plus the value of Lmax for this nuclide) are required. 2. Lmax is the maximum value of the orbital angular momentum. 3. If a second equal sign is present, the integer value following that equal sign is the number of fission channels to be included. 	No
12,13		Repeat lines 9 and 10 for this nuclide	
14 ...		Repeat lines 11 through 14 as needed	