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EVALUATION OF CHARGED-PARTICLE REACTIONS FOR FUSION APPLICATIONS

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Abstract: New evaluations of the total reaction cross sections for ^{2}H(d,n)^{3}He, ^{2}H(d,p)^{3}H, ^{3}H(t,2n)^{4}He, ^{3}H(d,n)^{4}He, and ^{3}He(d,p)^{4}He have been completed. These evaluations are based on all known published data from 1946 to 1990 and include over 1150 measured data points from 67 references. The purpose of this work is to provide a consistent and well-documented set of cross sections for use in calculations relating to fusion energy research. A new thermonuclear data file, TDF, and a library of FORTRAN subprograms to read the file have been developed. Calculated from the new evaluations, the TDF file contains in rmation on the Maxwellian-averaged reaction rates as a function of reaction and plasma temperature nd the Maxwellian-averaged average energy of the interacting particles and reaction products. Rout es are included that provide thermally-broadened spectral information for the secondary reaction products.

[^{2}H(d,n)^{3}He, ^{2}H(d,p)^{3}H, ^{3}H(t,2n)^{4}He, ^{3}H(d,n)^{4}He, ^{3}He(d,p)^{4}He reactions, charged-particle evaluations, sion reactions, fusion reactivities, Maxwellian-averaged reaction rates, calculated emission spectra, astrophysical S-factors, R-matrix analyses]

Introduction

This work has been done to provide a consistent and well-documented set of evaluated cross sections from which processed information can be generated for use in fusion applications. An important part of this is to provide the user with a realistic assessment of the uncertainties remaining in these reaction cross sections. We have developed a processed data file which accurately represents the information needed in practical calculations. *This paper contains only the most brief summary of an extensive final report to be produced later this year* and is referenced here as LLNL evaluation [91].

We have assessed and extracted total reaction cross sections as a function of energy. The sources of experimental data were in the form of integrated cross sections, angular distributions of secondary particles, measurements at one angle multiplied by 4π where the angular distribution is assumed or known to be isotropic, or, astrophysical S-factors—basically a quantity which is the cross section divided by the Coulomb penetrability and incident energy. It is usually smoothly varying with energy and represents the nuclear part of the cross section. Some data sets were available only in graphical form and were scanned with a digitizing program written for this application to insure that no additional error (beyond that introduced by the draftsman) resulted. Integrated cross sections were obtained from measured angular distributions by converting them to center-of-mass values and using a least-squares fitting procedure to obtain Legendre polynomial coefficients according to a consistent prescription.

Cross section evaluations

References and graphical symbols for the experimental data bases used in the five evaluated reaction cross sections are given in Figs. 1, 4, 8, 10, and 14 and in the references section. Also included in these figures are the uncertainties (at the 95% confidence level) we place on the evaluations *over the energy range of importance to fusion applications.*

In Fig. 2, we show the two most recent measurements of the ^{2}H(d,n)^{3}He reaction by Brown[90] and Krauss[87] along with the older measurement of Arnold[54] plotted in terms of the astrophysical S-factor from E_d=0 to 0. 2 MeV (in all figures the scale is the kinetic energy of the cident particle in the laboratory frame). The measurements of Krauss[87] are separated into (b) and (m) because they were carried out at two different facilities. The measurements of Brown[90] are approximately 8% higher than the previous measurements. In Fig. 3, an extrapolation of the S-factor from higher energies clearly favors the measurements of Brown[90]. Current knowledge of the structure of ^{4}He indicates that the S-factor is smooth over the 400 keV range plotted in Fig. 3. Not shown in Fig. 3 are the data of Davidenko[57] because of a shape difference and large error bars and the data of Chagnon[56] which are considerably different from the other measurements. As with the other reactions discussed below, data of some authors listed in Fig. 1 for the ^{2}H(d,n)^{3}He reaction are not shown because they are not in the energy range plotted in the figure.

In Fig. 5, we show all the data for the ^{2}H(d,p)^{3}H reaction from E_d=0 to 0.2 MeV. The data are somewhat discrepant but an extrapolation of the S-factor from higher energies together with the data of Brown[90] and Arnold[54] and knowledge of the structure of ^{4}He give us confidence in the evaluation to ±3%. In Fig. 6 we show the high energy evaluation of the ^{2}H(d,p)^{3}H reaction as the S-factor vs. E_d. Plotted in this way, an extrapolation to 30 MeV is less difficult to make. Figure 7 shows the same data plotted in terms of cross section vs. E_d.

The data base for the ^{3}H(t,2n)^{4}He reaction is more sparse as can be seen in Figs. 8 and 9. The S-factor vs. E_t shows a clear indication of changing slope from E_t=0 to 0.4 MeV. The evaluation above 1 MeV is heavily weighted in favor of the measurements of Govorov[62] and Jarmie[58]. Further details describing this evaluation will be given in the final report.

The ^{3}H(d,n)^{4}He reaction evaluation shown in Fig. 11 is based on a single-level R-matrix fit to all but three measurements. The three data sets not used are shown in

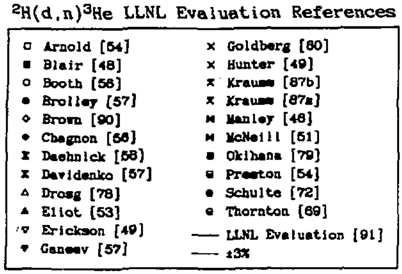

Fig. 1. References and plotting symbols used for the $^2H(d,n)^3He$ reaction data as shown in Figs. 2 and 3.

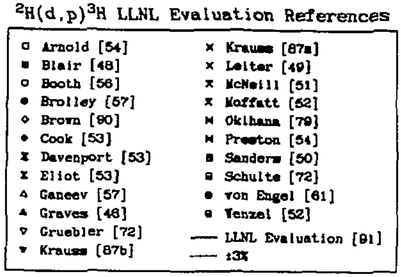

Fig. 4. References and plotting symbols used for the $^2H(d,p)^3H$ reaction data as shown in Figs. 5, 6, and 7.

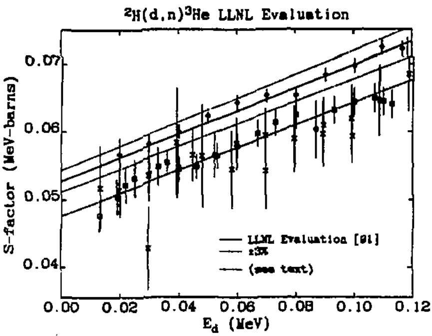

Fig. 2. The recent measurements of Brown[90] and Krauss[87] are plotted with the work of Arnold[54] as the astrophysical S-factor vs. E_d in the laboratory frame. The data of Brown[90] are approximately 8% higher than the previous measurements.

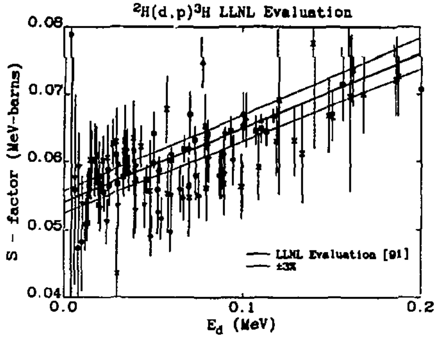

Fig. 5. All $^2H(d,p)^3H$ experimental data and the evaluation plotted as the S-factor vs. E_d from 0 to 0.2 MeV.

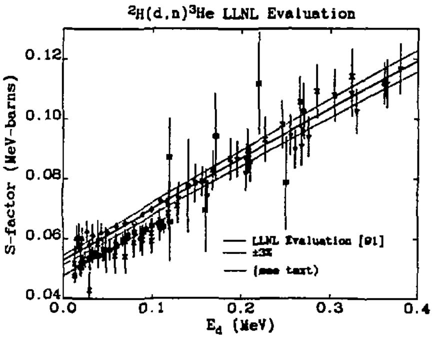

Fig. 3. The dashed line here and in Fig. 2 represents the most likely evaluation in the energy range E_d=0 to 0.12 MeV without the Brown[90] measurement and if no data had existed above 0.12 MeV. Not all data are plotted in this figure (see text).

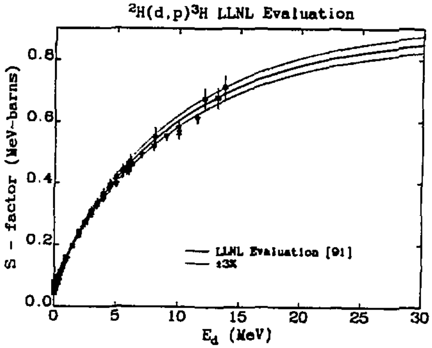

Fig. 6. Data and the evaluation of the high-energy portion of the $^2H(d,p)^3H$ reaction plotted in terms of the S-factor vs. E_d to show how the evaluation was carried out to 30 MeV.

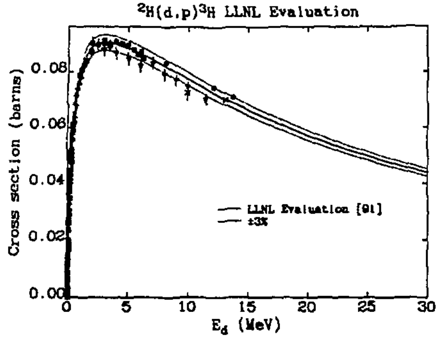

Fig. 7. Same as in Fig. 6 except plotted as cross section vs. E_d to show how the cross section is extrapolated to 30 MeV.

Fig. 12 as ratios to the evaluation with the dashed lines serving to guide the eye. Numerous R-matrix calculations were performed using many energy ranges and using various subsets of all the data. All of the results fall within the ±2% indicated. The final evaluation is based upon allowing the normalization of each measurement to vary while simultaneously performing a least-squares fit with a single-level R-matrix calculation. Shown in Fig. 11 are the measurements used in the R-matrix fit, the average percent error for each data set, and the percent change in the overall normalization for arriving at the best fit. We assumed that the overall normalization of the entire data base is roughly correct and therefore the normalizations of the individual data sets were allowed to vary subject to the constraint that the average normalization was unity. The data plotted in Figs. 11 and 12 have been renormalized by the amount indicated in Fig. 11. In Fig. 13, we show the R-matrix analyses by Jarmie[84] and Brown[87] as ratios to the LLNL evaluation [91]. We also show the effect of not allowing the individual data sets to change in normalization. All of these results fall within ±2% and indicate to us the uncertainty limits of this data base. More specific details of the R-matrix calculations and renormalization procedures will be presented in the final report.

Of the five reactions evaluated in this work, the measurements for the ^{3}He(d,p)^{4}He reaction (Fig. 15) are the most discrepant. The absolute values differ by more than the experimenters' quoted errors. As shown in Fig. 16, except for the data sets of Bonner[52] and Jarvis[53] and the low-energy portion of the data sets of Carlton[70] and Kliucharev[56], the shapes are in good agreement. For E_d=0 to 800 keV, the evaluation is based on a single-level R-matrix fit to all the available data except for those discussed above. Many R-matrix calculations were performed under a variety of conditions and the best fit was obtained by simultaneously allowing the individual data set normalizations to vary. The normalizations of many data sets differ with one another by more than the quoted errors and it is not obvious which measurement is correct. Therefore, we assumed that, on the average, the overall normalization of all the measurements is correct and the individual data set normalizations should average to unity. In Fig. 17, we show the average percent error for each data set and the percent change in normalization for arriving at the best fit. The data plotted are only those points included in the fitting process and have been renormalized by the indicated amounts. We believe the evaluation to be good to no better than ±8% in normalization even though we are certain that the shape of the ^{3}He(d,p)^{4}He reaction is known much better.

Applications File—TDF

We have developed a thermonuclear data file, TDF, which is an ASCII file that contains thermonuclear reaction rates and spectral information on the outgoing particles as a function of plasma temperature. This file contains interpolatable data for all plasma temperatures from 100 eV to 1 MeV. It is assumed that the distribution of the reacting particles in the plasma is Maxwellian. Currently, TDF contains reaction rates and spectral information calculated

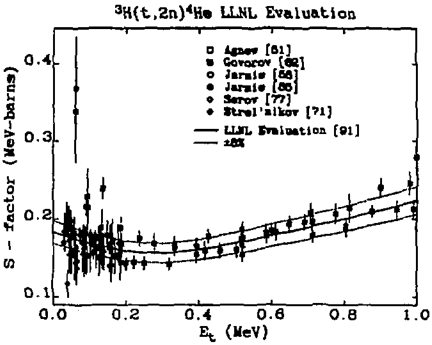

Fig. 8. Plot of all experimental data and evaluation of the ^{3}H(t,2n)^{4}He reaction from E_t=0 to 1.0 MeV. The change in slope of the evaluation between 0 and 0.5 MeV is independent of any particular data set or of the evaluation techniques we used on this data base.

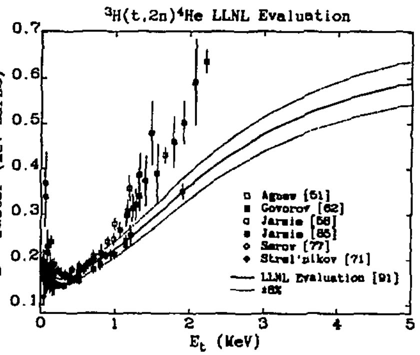

Fig. 9. Plot of the ^{3}H(t,2n)^{4}He data and extrapolation of the evaluation to higher energies in terms of the S-factor vs. E_t. Further details describing this evaluation will be given in the final report described in the text.

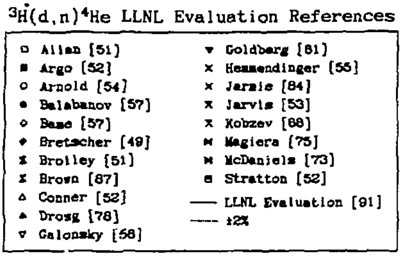

Fig. 10. References and plotting symbols used for the ^{3}H(d,n)^{4}He reaction data as shown in Figs. 11, 12, and 13.

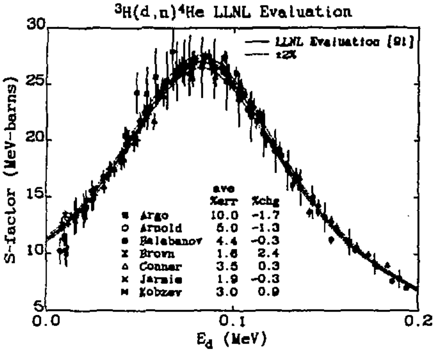

Fig. 11. Experimental data and evaluation for the ^{3}H(d,n)^{4}He reaction in terms of the S-factor vs. E_d. The *ave %err* is the average total error of each data set. The *%chg* is the renormalization of each data set for the best R-matrix fit (see text).

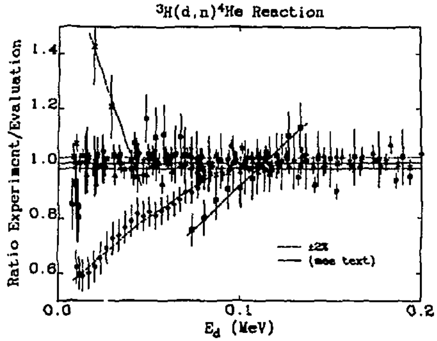

Fig. 12. Ratio of experimental data to evaluation for the ^{3}H(d,n)^{4}He reaction showing which data sets were excluded from the R-matrix fitting procedure.

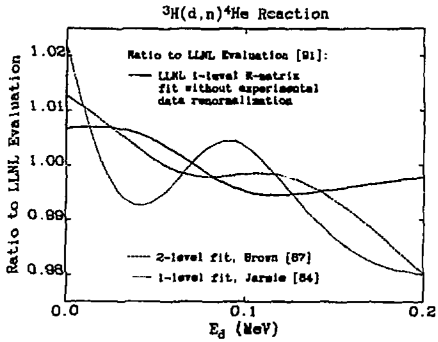

Fig. 13. Ratio comparisons of our R-matrix fit without data renormalization and the R-matrix fits of Jarmie[84] and Brown[87] to our evaluation of the ^{3}H(d,n)^{4}He cross section.

from the five evaluated reactions discussed in the previous section in units selectable by the user.

We have also developed a library of four subprograms written in FORTRAN77 for accessing TDF. The first subprogram is simply a reader and is called only once in an applications program prior to any call of the other three subprograms. The second subprogram returns the value of the reactivity (Maxwellian-averaged reaction rate) given a reaction number and a plasma temperature. The third subprogram returns the reactivity and the Maxwellian-averaged average energies of the two interacting particles and the reaction products given a reaction number and a plasma temperature. The fourth subprogram is a spectral lookup routine (SPECLU) which is slightly more complicated. This subprogram will return the energy of a secondary reaction particle and the value of the corresponding spectral shape function in the frame of a laboratory detector as a function of a real number, RN, between 0 and 1. We show in Fig. 18 plots of the normalized spectral distributions vs. neutron emission energy for the ^{3}H(d,n)^{4}He reaction at temperatures of 5, 10, 20, and 50 keV. These plots were generated by repeated calls to SPECLU for 1000 input RN's equally spaced between 0 and 1. The filled diamonds are the result of a CALL SPECLU as described above but for 2500 random numbers, RN, where the neutron energies are grouped into 50 bins. This gives one example of how this routine and TDF could be used in a Monte Carlo type calculation.

The calculations for the spectral information are carried out during the production of the TDF file so the file itself contains spectral data which lend themselves to fast look-up techniques. Because this information is obtained from complex calculations using the more fundamental cross sections, considerable effort was put into the computational algorithms to insure accuracy first and then speed. The processing code which produces the TDF file and the subprograms which provide the interpolations and look-ups introduce errors at a level of not more than 0.1%. The TDF file and the library of subprograms have been successfully tested on computers using three different operating systems and we consider them to be machine-independent. They will be available for public distribution later this year.

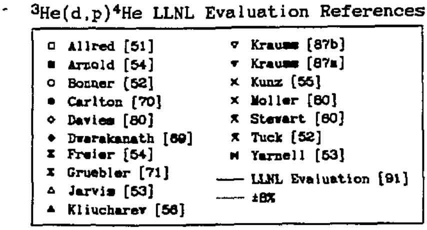

Fig. 14. References and plotting symbols used for the ^{3}He(d,p)^{4}He reaction data as shown in Figs. 15, 16, and 17.

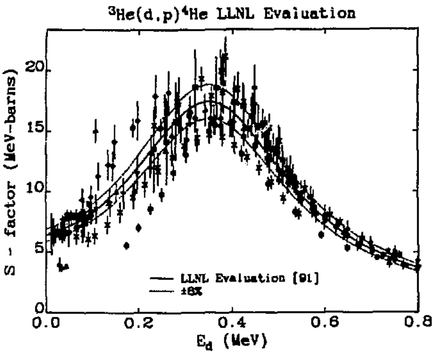

Fig. 15. Plot of all experimental data and evaluation of the ^{3}He(d,p)^{4}He reaction in terms of the S-factor vs. E_d from 0 to 0.8 MeV.

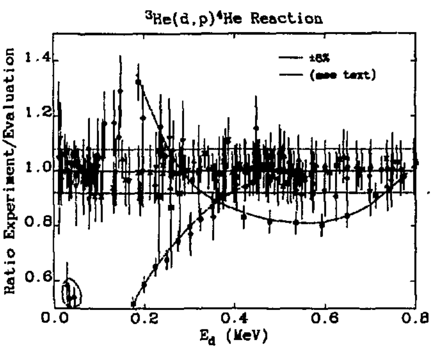

Fig. 16. Ratio of experimental data to evaluation for the ^{3}He(d,p)^{4}He reaction showing which data sets were excluded from the R-matrix fitting procedure.

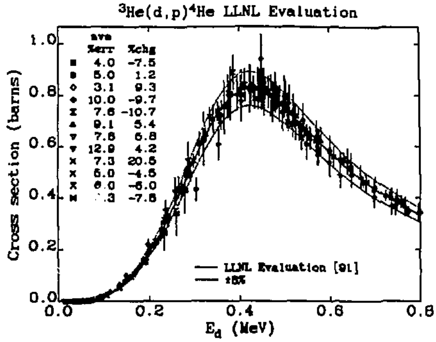

Fig. 17. Experimental data and evaluation for the ^{3}He(d,p)^{4}He reaction in terms of cross section vs. E_d. The numbers have the same meaning as described in Fig. 11.

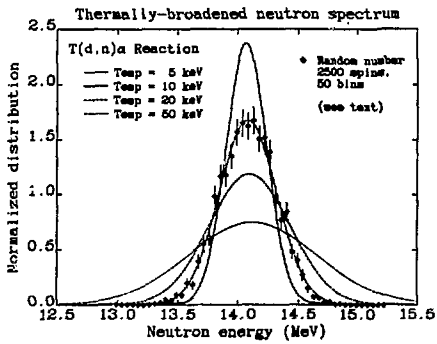

Fig. 18. Plot of the thermally-broadened neutron spectrum for the ^{3}H(d,n)^{4}He reaction for several plasma temperatures. The filled diamonds are described in the text. This information is obtained directly from TDF using the subprograms library.

Conclusions

We have given a brief overview of new evaluations of the most important charged-particle reaction cross sections needed for current fusion applications. We have also discussed a new applications file, based on these evaluations, which is machine-independent and provides the most important kinds of information necessary for fusion applications. This paper is intended to provide only a brief summary of a more extensive report to be produced later this year.

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