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PROGRESS REPORT

Applied Nuclear Data Research and Development Quarterly Progress Report

for the Period
July 1 through September 30, 1973

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

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Edited by

D. R. Harris, Group Leader
Nuclear Data Group, T-2

This work performed under the joint auspices of the U.S. Atomic Energy Commission's Divisions of Military Applications, Reactor Research and Development, and Controlled Thermonuclear Reactors, as well as the Defense Nuclear Agency of the Department of Defense, and the National Aeronautics and Space Administration.

ABSTRACT

This report presents progress in provision of nuclear data for nuclear design applications. The work described here is carried out through the LASL Applied Nuclear Data Group and covers the period July 1 through September 30, 1973. The topical content of this report is summarized in the Contents.

CONTENTS

APPLIED NUCLEAR DATA RESEARCH AND DEVELOPMENT

I. MULTIGROUP PROCESSING CODE, MINX (C. R. Weisbin, P. D. Soran, J. S. Hendricks, R. J. LaBauve, and D. R. Harris)

The multigroup processing code MINX is being developed to enable the user to obtain multigroup sets known to be accurate to within an input specified tolerance, provided one assumes that the data base and weighting functions are known explicitly. It is a designer-oriented processing code with improved resonance and group-to-group transfer capabilities. All pertinent ENDF/B formats are considered and a pseudo-composition independent multigroup library with self-shielding factors is generated in CCCC[1] format.

During the past quarter, implementation of a treatment of the unresolved resonance region was begun and about 90% completed. This treatment is one that was agreed upon at a meeting held at GE (Sunnyvale, California) on June 26-27, 1973 which was attended by personnel from Los Alamos Scientific Laboratory, General Electric, Lawrence Livermore Laboratory, and Brookhaven National Laboratory. The treatment is essentially that now incorporated in the ETOX[2] code.

Coding for producing MINX output in CCCC[1] format is now about 90% complete.

Two studies were conducted using the MINX code to determine relative importance of weighting functions and group structure design in a multigroup averaging code. In the first study,[3] a very fine group structure[4] was chosen and f-factors were computed for three different weighting functions. The results shown in Table I indicate that for a sufficiently fine group structure, the f-factor calculation is essentially independent of the input weighting function.

In the second study[5] the multiplication factor of a reference system[6,7] was computed using three different multigroup structures, three different weighting functions, and three different processing codes (MC-2,[8] ETOG,[9] and MINX).

The results shown in Table II clearly demonstrate the strong effect of the weighting function on a coarse group problem.

II. EVALUATION OF THE NEUTRON-INDUCED CROSS SECTIONS FOR ^{10}B (P. G. Young, G. M. Hale, D. G. Foster, Jr., and D. M. McClellan)

An evaluation of the neutron-induced total, elastic, inelastic, (n,p), (n,d), (n,t), and (n,α) cross sections for ^{10}B has been completed for neutron energies of 2-20 MeV. The elastic angular distributions and gamma ray production cross sections have also been determined over the same energy region. The evaluation is based mainly on experimental data, although optical model and Hauser-Feshbach calculations were used to estimate shapes for (n,n') reactions to certain levels and to extend the elastic angular distributions from 14 to 20 MeV. The evaluated data are in ENDF/B format and will be attached to the R-matrix analysis below E_n = 2 MeV which is in progress.

III. NUCLEAR DATA FOR BUILDUP, TRANSMUTATION, AND DECAY OF FISSION PRODUCTS (T. R. England)

Initially motivated by questions on the magnitude of after-heat in reactor safety raised during the 1972-73 Emergency Core Cooling Systems Hearings (ECCS), a task force was organized to review, update, and extend the national nuclide data base (ENDF/B-IV) for use in programs such as CINDER, RIBD, and ORIGEN. This effort includes evaluation of fission fragment yields, cross sections, branching ratios, decay constants, decay energies, new ENDF/B formats, and related aspects such as specification of integral benchmark experiments.

The first compilation of data encompasses 823 nuclides. It will now include line spectra, light and heavy nucldies, and nuclides of interest in CTR and weapons applications. The ultimate use of these data is now intended to include studies of fallout, absorption, decay heat, fuel and waste management,

TABLE I

Average Percent Deviation for Infinitely Dilute Cross Sections and f-factors Obtained for Constant, 1/E and 1/E + Fission Spectrum Smooth Bondarenko Weighting*

	σ(0°,∞)	f(2100°,∞)	f(300°,50)	f(2100°,50)	f(300°,0)
Pu^{239}					
total	.187	.036	.137	.097	.166
elastic	.118	.011	.072	.056	.082
(n,2n)	.127	.000	.000	.000	.000
fission	.257	.031	.058	.055	.090
1st level	.056	.001	.001	.001	.001
capture	.290	.029	.078	.073	.115
Fe					
total	.152	.007	.016	.014	.069
elastic	.159	.003	.006	.008	.032
(n,2n)	.557	.000	.000	.000	.001
1st level	.081	.005	.002	.002	.010
capture	.253	.006	.616	.006	.016
U^{235}					
total	.188	.026	.082	.070	.123
elastic	.029	.004	.009	.008	.010
(n,2n)	.224	.000	.000	.000	.000
fission	.225	.028	.057	.048	.087
1st level	.197	.001	.000	.001	.001
capture	.276	.031	.044	.049	.086

*Computations performed in proposed[1] CSEWG group structure

TABLE II

MULTIPLICATION FACTORS AS A FUNCTION OF NEUTRON MULTIGROUPS, WEIGHTING FUNCTION MODEL AND MULTIGROUP PROCESSING CODE

Number of Groups	A MC^2	B MINX MC^2 Weight	C ETOG MC^2 Weight	D MINX 1/E Fission	E ETOG 1/E Fission	F MINX Flat	G ETOG Flat
50	0.9964	-	-	-	0.9888	-	0.9899
36	1.0008	0.9959	0.9987	0.9561	0.9622	0.9651	0.9709
12	0.9846	0.9996	1.0019	0.6223	0.6295	0.6926	0.7082

shielding, etc.; in general, it will be used for a wide range of problems of interest to LASL.

A French group previously launched a similar massive effort to incorporate nuclide data into a format identical to ENDF/B where possible. Their work to date covers 622 nuclides in the range $^{71}Z_n$ to $^{170}Y_b$ and includes, in addition to the usual nuclide parameters, the detailed transition probabilities per γ emitted. That work was summarazed at the IAEA Paris Symposium in March, 1973.[10] A previously obtained tape of their data was defective and a corrected version is now available at LASL. This will serve as the basis for many decay energies for ENDF/B-IV in a modified form; approximately 300 of these nuclides have been identified as being of particular importance in fast and thermal reactors and will receive independent review.

Sixty nuclides requiring reaction cross sections to isomeric states have been identified and reported (Los Alamos Scientific Laboratory internal document T-2-L-727 dated September 21, 1973).

Fission yields, independent and cumulative, constitute the largest obvious uncertainty in the ENDF/B-IV decay file. Because of this, correspondence with task force members, including reviews and input to the ENDF/B-IV yields, has been necessary. This includes the active participation of LASL's CNC-11 group (K. Wolfsberg, Task Force consultant). In conjunction with CNC-11 a proposal to measure currently needed independent yields and improve the currently used model estimators for yield distribution is in preparation.

In conjunction with LASL's group P-2, a draft proposal has been prepared for accurate integral measurements of short term β and γ decay heating to be used, along with existing long cooling term absorption and heating data, in evaluation of the ENDF/B-IV nuclide data.

In support of these proposals, all known errors in our existing decay heat library have been corrected and many preliminary calculations for various fuels and irradiation conditions are completed. In addition, the massive amounts of new ENDF/B-IV data are being accumulated for general use at LASL and in anticipation of a requested data evaluation by the Division of Reactor Research and Development of the United States Atomic Energy Commission.

A code for data handling to be used with CINDER has been prepared; this code, or an independent one, requires expansion to process the ENDF/B-IV data into forms usable by CINDER, RIBD, and ORIGEN.

IV. PROCESSING OF ENDF/B TO GENERATE A POINTWISE EVALUATED NUCLEAR DATA FILE (PENDF) - THE ETOPL CODE PACKAGE (R. J. LaBauve, C. R. Weisbin, R. E. Seamon, M. E. Battat, D. R. Harris, and P. G. Young)

Progress was made in three major areas in the ETOPL (ENDF/B to pointwise library) code package during the last quarter. First, a routine was added for expressing the gamma-ray production data in a format more suitable for use as a Monte Carlo data base. In this format, the gamma-ray production cross sections and gamma-ray spectra for all reactions are combined and expressed as a single isotropic, non-elastic reaction. The gamma-ray production cross sections for this reaction are given on the same energy mesh as the neutron reactions.

Second, routines were added for preparing additional tables in the unresolved region for the total, elastic scattering, fission, and capture cross sections. These tables give the cross sections as a function of the self-shielding parameter, σ_0, and are necessary for Monte Carlo application as the current versions of MINX and the ETOPL code package calculate cross sections in the unresolved resonance region from average parameters.

Finally, an improved thinning technique[11] is being incorporated into the LUST segment of the ETOPL code package as an alternate option to the "three-point" algorithm currently in the code. The older procedure suffers from a number of deficiencies. For example, only every other point is thinned from a set of points lying on a straight line. The new method reproduces the significant structure of each cross section while averaging ripples in the data of the order of magnitude of the error tolerance.

V. TESTING OF NUCLEAR DATA OF IMPORTANCE IN SHIELDING, APPLICATIONS AGAINST INTEGRAL EXPERIMENT (R. J. LaBauve and D. W. Muir)

Calculations are continuing on the gamma-ray portions of the ZPPR/FTR-2 shield experiment.[12] Good agreement was obtained[13] between calculated and experimental neutron reaction rates for that experiment. However, in our first attempt to calculate the gamma-ray dose distributions, a rather large discrepancy was observed in the region of the reactor core. This problem has been investigated and found to be due to a normalization error in the constructed source of gamma-rays due to fission product decay. A recalculation of the gamma-ray transport and the resulting dose distributions, using the corrected source, is now in progress.

VI. NUCLEAR DATA FOR THE CONTROLLED FUSION PROGRAM (D. W. Muir, L. Stewart, R. J. LaBauve and T. R. England)

Work has continued on the development of a multigroup neutron activation library for the calculation of decay heating and radiological hazards in the Reference Theta Pinch Reactor (RTPR). This collection of activation data, called the LASL/CTR activation library, has been written onto a magnetic tape which is arranged identically to the tape containing the LASL/CTR neutron/photon transport cross section library. A short computer program BARGRAF has been written to prepare histogram plots of the multigroup data contained in two CTR design libraries. These plots not only display the data, but they also allow for visual check for obvious errors.

The Cross Section Evaluation Working Group (CSEWG) decided in May to incorporate a 14-MeV fusion peak in the standard weighting function to be used in conjunction with the 239-group fast neutron standard group structure.[4] Since we have been using such a fusion peak in fusion reactor and weapons-related cross section processing, we were asked to review the shape of the thermonuclear peak and to present recommendations to the committee. The results of this study will appear in a report[14] which contains a derivation of the Gaussian peak shape, a review of fusion reactor plasma temperatures, and numerical examples which illustrate the sensitivity of spectrum-averaged cross sections to the plasma temperature. Based on this study, a "typical" plasma temperature of 20 keV (which gives a peak-width of 790 keV) was recommended to CSEWG. For most cases of interest, deviations of the actual plasma temperature from this value are not expected to cause serious errors in group constants obtained using the 239-group structure.

L. Stewart and D. J. Dudziak hosted the meeting of the Controlled Thermonuclear Research Subcommittee of the U. S. Nuclear Data Committee at Los Alamos Scientific Laboratory on September 11-12. Minutes will be available when they have been finalized and approved by the parent USNDC, which is an advisory committee to the Atomic Energy Commission.

VII. EVALUATION OF NEUTRON AND GAMMA RAY PRODUCTION CROSS SECTIONS FOR ^{14}N (P. G. Young, D. G. Foster, Jr., G. M. Hale, and D. M. McClellan)

The revisions of the ^{14}N evaluation described in our previous progress report have been incorporated into LASL nculear data files, and the new data set is available from the DNA Military Applications Nuclear Data Library at the Radiation Shielding Information Center as MAT 4133, MOD4. The new evaluation has also been submitted to the National Neutron Cross Section Center at Brookhaven National Laboratory for inclusion in Version IV of the national nuclear data file ENDF/B. It has been determined that this ^{14}N evaluation will be employed in the next round of calculations on SPRINT nuclear environments.

VIII R-MATRIC ANALYSIS OF REACTIONS IN THE ^{17}O SYSTEM (G. M. Hale, P. G. Young, and D. G. Foster)

The extension of our multichannel, multilevel R-matrix analysis of the reactions $^{16}O(n,n)^{16}O$, $^{16}O(n,\alpha)^{13}C$, $^{13}C(\alpha,\alpha)^{13}C$ to neutron energies below 6 MeV was completed in this quarter. The results have been incorporated in part in a Defense Nuclear Agency (DNA) sponsored evaluation of neutron induced reactions on oxygen at energies up to 20 MeV.

The level scheme of Johnson,[15] which was followed closely in this analysis, appears to be consistent with the data from all three reactions in this energy range, except for two isolated regions where differential cross section data indicate the need for revised assignments. Alternative assignments are presently being tried for resonances in these regions.

At a recent meeting held at LASL, the DNA expressed strong interest in attaching complete, if crudely estimated, error files to evaluations done with its support. These files are to contain both the variances of the cross sections and the covariances among the cross sections in the evaluated data set. The covariances, in particular, are important to obtain the variance-covariance matrices for group cross sections that are used in sensitivity studies of thick geometry configurations. The variance-covariance matrix supplied for the resonance parameters by our R-matrix fitting code (EDA) can be used to calculate analytically variances and covariances for the predicted (evaluated) cross sections. We are currently generating these numbers in the case of the oxygen evaluation to gain insight into the systematics of these correlations for resonant structure in the cross sections.

IX. RE-EVALUATION OF NEUTRON-INDUCED CROSS SECTIONS OF ^{16}O (P. G. Young, D. G. Foster, Jr., G. M. Hale, R. A. Nisley, and D. M. McClellan)

Extensive revisions have been made to our previous ENDF/B-III evaluation of neutron-induced cross sections of ^{16}O. The most important changes follow.

The results of an R-matrix analysis were incorporated into the total, elastic scattering, and (n,α_0) cross section files and into the elastic angular distribution files below E_n = 5.7 MeV.

Adjustments were made to the (n,n') level excitation cross sections, particularly the (n,n') to the first excited state of ^{16}O, so that the evaluated data agree better with the elastic and (n,n') measurements of Kinney and Perey[16] and Nellis and Buchanan.[17]

The elastic angular distributions between 6 and 9 MeV were modified to agree better with the measurements of Kinney and Perey.[16]

Inelastic scattering angular distribution measurements to the first five excited states of ^{16}O for 14-MeV neutrons were analyzed, and anisotropic angular distributions were introduced into the evaluation above E_n = 10 MeV.

Angular distribution measurements for the 6.131- and 6.917-MeV gamma rays from inelastic neutron scattering were analyzed, and anisotropic distributions were added to the evaluation.

The cross section and Legendre coefficient files were systematically thinned at all energies.

The revised data are available from the DNA Military Application Nuclear Data Library at RSIC as MAT 4134, MOD2. The data also have been submitted to the National Neutron Cross Section Center (NNCSC) for inclusion in Version IV of the national nuclear data file ENDF/B.

X. MEDIUM AND LOW ENERGY CROSS SECTION LIBRARY (D. G. Foster, D. R. Harris, and N. L. Whittemore)

A program is under way to improve the accuracy and cost-effectiveness of medium and low energy particle and photon transport calculations. The ENDF/B library of cross sections for neutrons and photons below 20 MeV is augmented by cross sections at higher energies for other particles. Required cross sections are determined from nuclear model cascade and evaporation calculations and from experimental data.

Nuclear model calculations were completed in the current quarter for protons up to 800 MeV on iron and molybdenum. A number of tapes containing equivalent nuclear model calculation data were consolidated for convenience and to release tapes.

Cross sections are provided both for neutrons and for charged particles, but it is of considerable interest to determine the degree to which neutron-only calculations suffice for applications ignoring the charged particles except in providing the neutron source and in creating neutron-induced effects.[18] For this purpose, the medium energy Monte Carlo transport code NMTC[19] has been modified to tag histories of neutrons which ever had a charged particle ancestor. Preliminary calculations with poor statistics suggest that relatively few neutrons below 800 MeV with charged-particle ancestors penetrate practical thicknesses of shielding materials.

XI. MULTIGROUP NEUTRON AND PHOTON CROSS SECTIONS FOR CADMIUM (R. J. LaBauve and D. W. Muir)

Gamma-ray production and transport cross sections were generated for cadmium for use in weapons vulnerability calculations. These 30-group (neutron) + 12-group (photon) cross sections were coupled to an existing four-table neutron cross section set to form a completely coupled (42 X 45 entries per table) four-table, neutron/gamma-ray cross section set for cadmium.

XII. REEVALUATION OF CROSS SECTION FOR $^{203}Tl(n,2n)^{202}Tl$ (D. W. Muir)

Cross sections have been reevaluated for the fast neutron monitor reactions $^{203}Tl(n,2n)^{202}Tl$. The excitation function for this reaction generally used in previous Los Alamos calculations is based on a 1961 measurement of Prestwood and Bayhurst,[20] extended smoothly down to an assumed reaction threshold of 8.8 MeV. The recent nuclear mass tables of Wapstra and Gove[21] indicate that the threshold should be about an MeV lower, at 7.8 MeV. This cross section was measured also by Tewes et al.[22] in 1960 and a remeasurement is in progress at Los Alamos.[23] The Tewes data are in good agreement with the preliminary data from the Los Alamos remeasurement, and both are consistent with the lower value of the reaction threshold. Thus our reevaluation of the excitation function for $^{203}Tl(n,2n)^{202}Tl$ follows the shape of the Tewes data rather than the 1961 Prestwood and Bayhurst data. This change nearly doubles the average cross section in the 9-13 MeV region, relative to the value at 14 MeV.

XIII THE $^{11}B(p,\alpha)^{8}Be$ CROSS SECTION AND SPECIFIC REACTION RATE (G. Hale, D. R. Harris, and P. G. Young)

The $p + {}^{11}B \rightarrow 3\,{}^{4}He + 8.68$ MeV reaction is of interest as a potential thermonuclear fuel system.[24] Nearly all the reaction products are safe, nonradioactive helium nuclei, and the side branches $^{11}B(p,\gamma)^{12}C$, $^{11}B(p,n)^{11}C$, $^{11}B(\alpha,n)^{14}N$ and $^{11}B(\alpha,p)^{14}C$ occur infrequently. The specific reaction rate $\langle\sigma v\rangle$ is large at temperatures of order 200 keV and in some evaluations of the cross section the $\langle\sigma v\rangle$ for this reaction exceeds that for DT, DD, and $D^{3}He$ at temperatures above 200 keV. We have evaluated the cross section for this reaction on the basis of existing experimental data and, for comparison with other evaluations, we have computed $\langle\sigma v\rangle$ for temperatures below 1 MeV. Our evaluation and computation of $\langle\sigma v\rangle$ is near or below the lower limit of previous evaluations at all temperatures. Because of the interest in this reaction, new measurements are in progress both at Cal Tech and at Lawrence Livermore Laboratory.

The $^{11}B(p,\alpha)^{8}Be$ reaction cross section to the ground state and to the first excited state of ^{8}Be were evaluated at energies up to 3 MeV. The ^{8}Be nucleus is unstable to breakup into two alphas, so three alphas are produced by both partial reactions. The results of the analysis for the combined (p,α_0) and (p,α_1) channels are presented in Fig. 1, together with the experimental data of Beckman et al.,[25] Symons and Treacy,[26] and Segel et al.[27] Below 0.82 MeV the evaluated curve represents an R-matrix calculation using the code EDA, based on the resonance parameters determined by Ajzenberg-Selove and Lauritsen.[28] At higher energies the evaluation is based primarily on the experimental data of Segel et al.[27]

The evaluated $^{11}B(p,3\alpha)$ specific reaction rate, integrated numerically over a Maxwellian distribution, is compared in Fig. 2 with specific reaction rates for important thermonuclear fuels. Also shown are values of $\langle\sigma v\rangle$ for $^{11}B(p,3\alpha)$ integrated by the method of steepest descent, an approximate integration technique which with corrections is widely used in the astrophysical literature.[29]

Figure 2 shows that the $^{11}B(p,3\alpha)$ specific reaction rate displayed by Weaver, Zimmerman, and Wood[24] lies well above our determination.

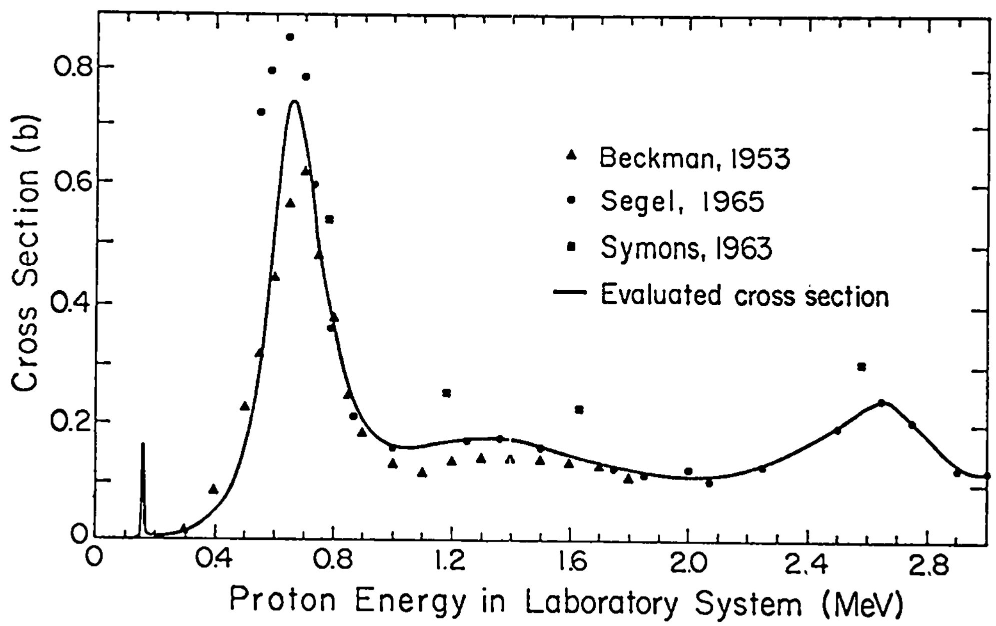

Fig. 1. The $^{11}B(n,\alpha)^{8}Be$ reaction cross section to the ground and first excited dates of ^{8}Be. The evaluation (solid curve) is compared to the experimental data of Beckman et al., Symons, and Treacy, and Segel et al.

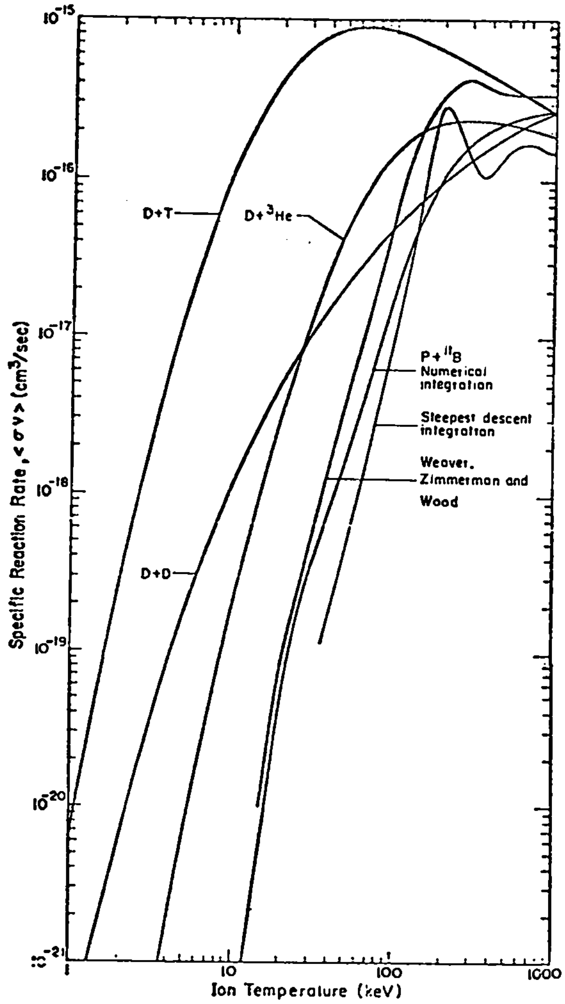

Fig. 2. The specific reaction rates for $p + {}^{11}B$ and other thermonuclear reactions. Converged numerically integrated values of $\langle\sigma v\rangle$ for $p + {}^{11}B$ are compared with the approximate integration by steepest descent.

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