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A BASIC EVALUATED NEUTRONIC DATA FILE FOR ELEMENTAL SCANDIUM

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ABSTRACT

This report documents an evaluated neutronic data file for elemental scandium, presented in the ENDF/B-VI format. This file should provide basic nuclear data essential for neutronic calculations involving elemental scandium. No equivalent file was previously available.

* This work supported by the United States Department of Energy under contract W-31-109-Eng-38; also under the auspices of The Physicist's Consultive, Downers Grove, Illinois.

I. INTRODUCTION

Elemental scandium (100% ^{45}Sc) is involved in nuclear applications (e.g., it is widely used as a fast-neutron filter due to sharp resonance windows [1]) In aspects of these applications it is important to carry out quantitative neutronic calculations. Such calculations require a comprehensive neutronic data base. Despite these facts, the national evaluated neutronic file system (ENDF/B-VI [2]) contains only a fragmentary scandium file, consisting largely of an assortment of dosimetry information. That file is devoid of such essential content as total and scattering cross sections, and it is certainly unsuitable for general neutronics calculations.

In order to provide a reasonable basic scandium evaluated file for neutronic calculations, this evaluation work was undertaken. It complements more fundamental studies of the fast neutron interaction with scandium at this laboratory reported elsewhere [3]. The available experimental data base is far from definitive, thus considerable reliance had to be placed upon calculational extrapolation. Where appropriate, remedial experimental and/or calculational work is suggested. With the limited experimental foundation, uncertainty estimates can be only qualitative. Furthermore, the user is cautioned that ^{45}Sc is near a double shell closure where "regional" and "global" calculational models may be less reliable [4].

This scandium file is expressed in ENDF/B-VI formats, it has passed routine checking procedures, and it has been forwarded to the National Nuclear Data Center, Brookhaven National Laboratory. Users interested in a copy of the numerical file should contact that Center. This is a neutronic file. Those requiring unusual information should consult special-purpose files (e.g., ref. [5]).

II. RESONANCE REGION

The representation of the resonance region extends up to ≈ 100 keV, explicitly using the parameters of ref. [6]. This is the same representation employed in the present ENDF/B-VI partial evaluation (MAT=2125). No adjustments were made to these parameters, and there may not be a perfect match to the energy-averaged cross sections extending to higher energies. In view of the various uncertainties involved, this should not be a serious shortcoming.

Subsequent to the resonance parameterization of ref. [6], used in the present evaluation, several large sets of resonance total-cross-section information have been reported. This new information should be used in a re-interpretation of the resonance parameterization of the low-energy interaction of neutrons with scandium. Such a re-interpretation is a specialized effort beyond the scope of the present work. However,

-- Recommendation:- Re-interpret the resonance region of scandium making use of the most recent experimental data sets.

III. NEUTRON TOTAL CROSS SECTIONS

There appear to be only four relevant scandium energy-averaged total-cross-section data sets in the literature. Two of these are comprehensive, extending from < 2 MeV upward [7,8]. A third set extends from ≈ 0.2 - 1.5 MeV [9], and a fourth [10] consists of only three isolated points. This very marginal experimental data base is shown in Fig. 1. The two primary data sets [7,8] are portions of major measurement programs that generally have proven to yield reliable results. However, in this instance, these two data sets are significantly discrepant in the several-MeV region. In view of the sparsity of information and the discrepancies, considerable reliance had to be placed upon the model predictions of ref. [11]. This model result very much supports the experimental results of ref. [7], and the shape is generally inconsistent with the measured values of ref. [8].

In view of the above unfortunate situation, the evaluation relies primarily upon the model calculations of ref. [11], slightly adjusted to improve the agreement with the measured values of ref. [9]. The model is founded upon detailed interpretations of elastic-scattering data. Below ≈ 1.5 MeV the evaluation follows an energy average of the detailed results of ref. [9]. The actual measurements portray a great deal of partly resolved fluctuations which are not represented in the evaluation. The evaluated result is compared with the experimental data base in Fig. 1. The uncertainties in the evaluated total cross sections are estimated to be several percent, but it is not realistic to quantify them with correlation matrices, etc. until better experimental data is available. There is no energy-averaged neutron total cross section of scandium in the ENDF/B-VI file for comparison.

-- Recommendation:- Measure energy-averaged scandium neutron total cross sections from 0.1 to 20 MeV with accuracies of ≲ 2%. At the lower extreme of this energy range, attention must be given to self-shielding effects and resonance structure. Such measurements are technologically feasible.

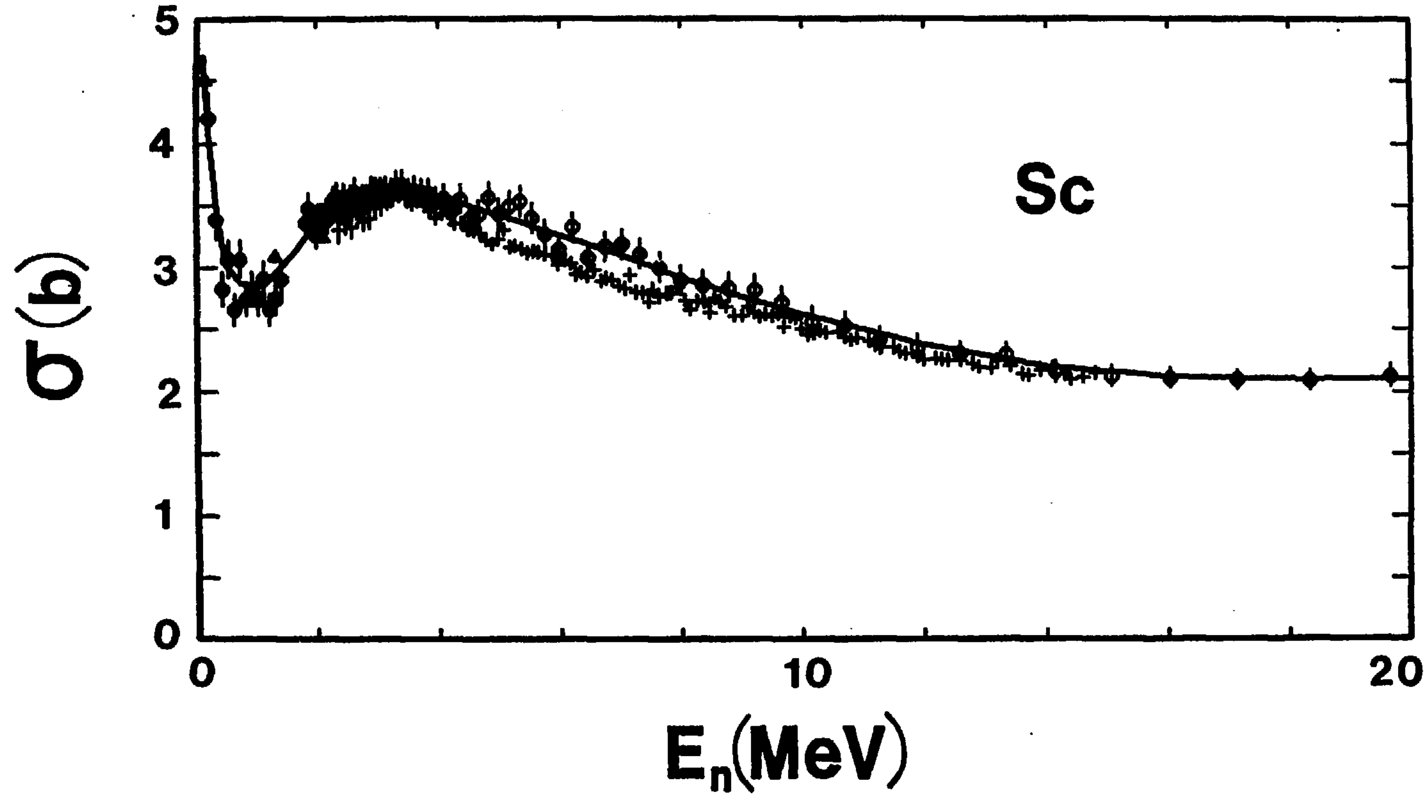

Fig. 1. Comparison of measured (symbols) and evaluated (curve) energy-averaged neutron total cross sections of elemental scandium. Energy averages of the experimental data sets are respectively indicated by: 0 = ref. [7], + = ref. [8], o = ref. [9], and Δ = ref. [10].

IV. NEUTRON SCATTERING

A. Elastic Processes

Elastic neutron scattering from scandium has been extensively studied, including measurements and model derivations, as reported in ref. [11]. None of the experimental work explicitly determines true elastic scattering as all of the measured elastic-scattering cross sections include inelastically-scattered contributions due to the excitation of the 12.4 keV first-excited level. However, the measurements do lead to a quantitative optical-statistical model which, in turn, can be used to extrapolate the measured values to true elastic scattering with reasonable reliability. That approach was used in deriving the present evaluated elastic scattering cross sections, using the model of ref. [11]. The model results were slightly adjusted to assure exact agreement with the above evaluated neutron total cross sections. These adjustments were largest at the very lowest energies where the work of ref. [9] clearly shows prominent fluctuating structure in the elastic-scattering cross sections. As in the case of the total cross sections, the evaluation follows the energy-averaged behavior of the elastic scattering cross sections above ≈ 100 keV, without attempting to reproduce the detailed and partially-resolved resonance behavior in the few-hundred keV energy region. Above 10 MeV, the evaluation depends entirely upon the model of ref. [11] as no experimental information is available.

The evaluated angle-integrated elastic-scattering cross section is illustrated in Fig. 2, together with the above total cross section and the implied non-elastic cross section. Up to ≈ 10 MeV, the evaluated elastic-scattering cross section is probably reliable to within several percent, but the uncertainty increases above 10 MeV due to the absence of any experimental information.

-- Recommendation:- Several good-quality differential elastic scattering measurements are needed between ≈ 10 and 20 MeV to confirm the energy behavior of the model used in the evaluation. Such measurements are technologically feasible.

The model of ref. [11] was also used to obtain the evaluated elastic-scattering angular distributions shown in Fig. 3. Again, these are supported by measurements only up to ≈ 10 MeV. The cross sections and the angular distributions are consistent with "Wick's Limit" [12]. The ENDF/B-VI scandium file contains no elastic-scattering information of any type for comparison.

B. Inelastic Processes

The knowledge of inelastic scattering due to excitation of discrete levels is discussed in detail in the companion document of

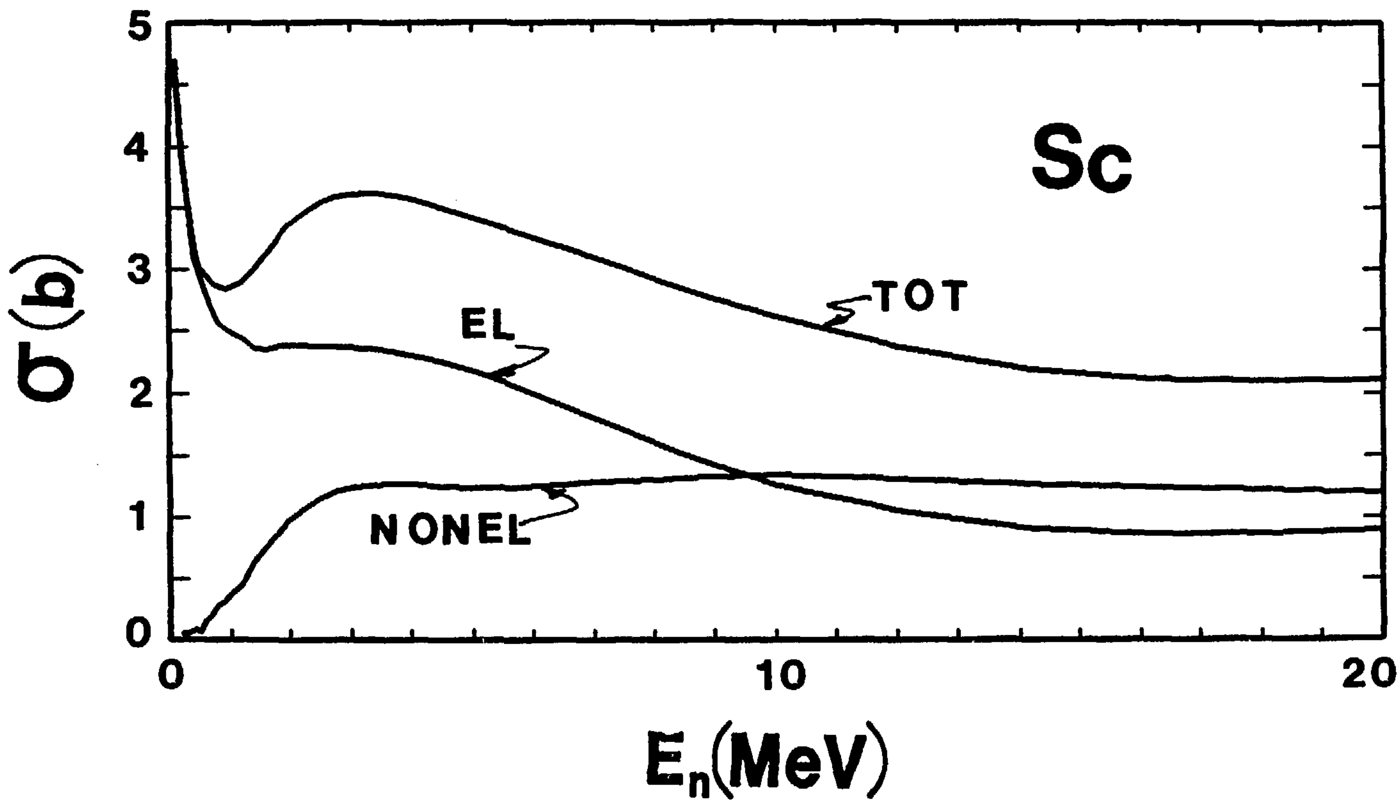

Fig. 2. Neutron total, elastic-scattering and non-elastic cross sections of scandium from the present evaluation.

ref. [11], including both experimental and calculational aspects of the process. The present evaluation employs the results of that study to provide the inelastic-scattering cross sections for the first 14 levels up to an excitation of ≈ 1.8 MeV. As pointed out in ref. [11], these excitations are primarily of a compound-nucleus nature with little observed anisotropy of the scattered neutrons. Therefore, the evaluation assumes isotropic scattered-neutron angular distributions. The first excited level in ^{45}Sc is at a very low energy (≈ 12.4 keV), with a corresponding threshold well below the upper-energy limit of the resonance portion of the present evaluation. This leads to a discrepancy between resonance total and partial cross sections and the energy-averaged cross section for the inelastic excitation of this first level up to incident energies of ≈ 100 keV. For the large majority of the applications, this discrepancy is of no note. Its mitigation would entail some extensive and uncertain resonance interpretations that are beyond the scope of the present work.

The onset of the continuum inelastic scattering cross section is at ≈ 1.8 MeV, and the magnitude is determined from the difference between the nonelastic cross section and the sum of the other partial reaction cross sections in the evaluation. It was assumed that the emitted neutron spectrum is isotropically distributed. That is little more than a qualitative approximation at higher energies as there will be an anisotropic pre-compound component. The continuum emission spectrum was taken from ref. [13], with small adjustments to assure internal file consistency. These continuum spectral distributions must be considered only approximations until such time as some substantive experimental information becomes available.

-- Recommendation:- Several double-differential neutron scattering measurements are needed, distributed over incident energies of 5 - 20 MeV, to define the evaluated continuum inelastic-neutron spectra. Such measurements are notoriously difficult above ≈ 10 MeV.

The above evaluated discrete inelastic-scattering cross sections are summarized in Fig. 4. The discrete inelastic-scattering cross sections are compared with the continuum inelastic scattering in Fig. 5. The latter is by far the larger over much of the higher-energy range. There is no inelastic-scattering information in the ENDF/B-VI scandium file for comparison.

V. NEUTRON RADIATIVE CAPTURE

The relevant experimental knowledge of the Sc(n,γ) cross sections is very limited and considerably discrepant [14-19]. All that can be reasonably concluded from these measurements is that the capture cross section is very small (few mbs) at energies of several-100 keV and

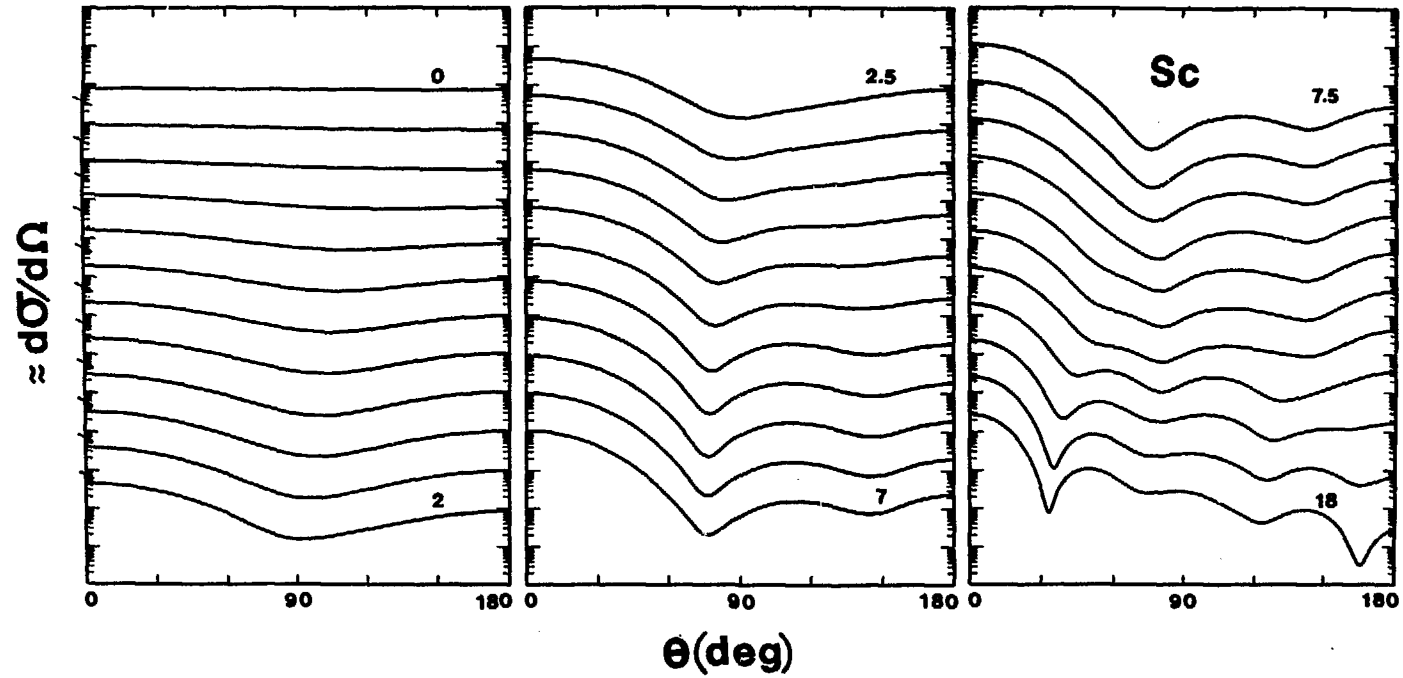

Fig. 3. Illustrative relative differential evaluated elastic-scattering cross sections from the present evaluation. Representative energies are noted numerically in MeV, with the distributions arranged in ascending order. The data are given in the laboratory coordinate system.

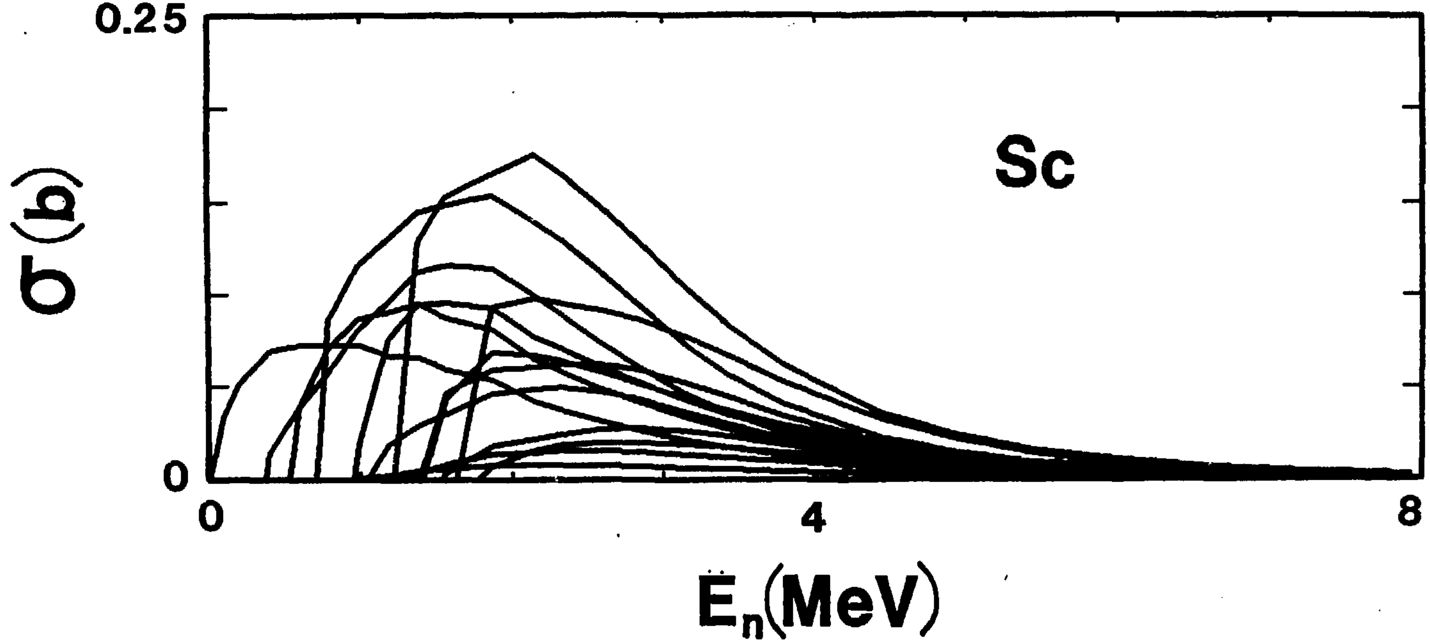

Fig. 4. Evaluated discrete inelastic-scattering cross sections of scandium as given in the present evaluation, and as described in ref. [11].

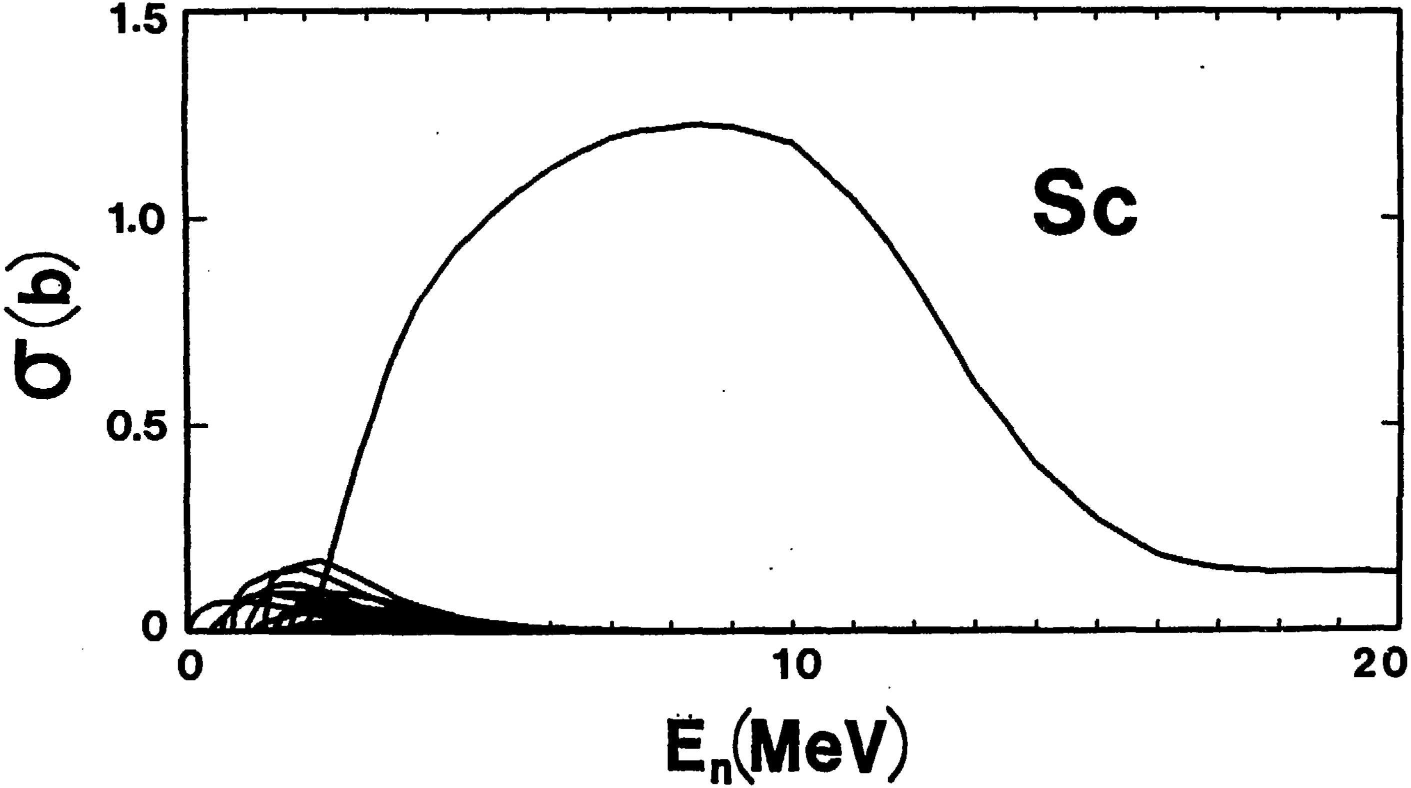

Fig. 5. Comparison of evaluated discrete inelastic-excitation cross sections with the large continuum contribution extending to 20 MeV.

above. With this unfortunate experimental situation, reliance had to be placed upon calculations to estimate the cross section values. Cross sections calculated with GNASH [20] and with ABAREX [21] were consistent to within 10 - 20%. The evaluation uses the ABAREX result, slightly adjusted at ≈ 100 keV in order to match the resonance region. The present evaluation is qualitatively consistent with that given in ENDF/B-VI except in the 0.5 - 1.5 MeV region where the latter has a shape that was not reproduced by any of the calculations. Even there the differences between the two evaluations are small (≲ 2.5 mb). The uncertainties in the evaluation may be as much as 50% or more. They will not be reduced without much improved experimental information. Therefore:-

-- Recommendation:- The Sc(n,γ) cross section should be measured with broad incident-neutron resolution from ≈ 100 keV to several MeV. The measurements will be tedious but are technically feasible, and accuracies of even 25% would be very useful.

VI. CHARGED- AND MULTIPLE-PARTICLE EMISSION

Relevant charged-particle thresholds [22] are given in Table VI-1, below.

Table VI-1. Scandium charged-particle emission thresholds.

Reaction	Threshold (in MeV)
(n,2n')	11.581
(n,3n')*	21.496
(n,p)	-0.526
(n;n',p)	7.044
(n,d)	4.770
(n;n',d)*	16.152
(n,t)	9.755
(n;n',t)*	17.865
(n,^{3}He)	11.594
(n;n',^{3}He)*	21.446
(n,α)	0.406
(n;n'α)	8.110

* These processes were ignored in the present evaluation as the threshold exceeds the upper (20 MeV) energy limit of the evaluation, or because the threshold energies approach that limit and the reaction cross sections are expected to be very small.

Some of these reactions lead to activities that may be useful for dosimetry purposes. The respective activation cross sections are not a part of this neutronic file. The user interested in activity information should consult a special purpose file such as that of ref. [5].

The experimental data relevant to the above reactions is generally sparse to non-existent. Therefore, considerable reliance had to be placed upon calculational estimate. The requisite calculations utilized the code GNASH [20] with the neutron potential of the companion document [11], the proton and ^{3}He potentials of Perey and Perey [23], the α potential of Wilmore [24], the deuteron potential of Lohr and Haeberli [25], and the triton potential of Becchetti and Greenlees [26]. The calculated results were adjusted to agree with experimental information where appropriate.

A. The (n,2n') Process

Metastable- (2.44 d) and ground-states (3.93 h) result from this process. Both have been extensively measured over more than thirty years, both decay modes in some cases [27 - 48]. Unfortunately, there is a wide variation in the various flux standards involved, the documentation is frequently scarce or non existent, and the results scatter widely. Renormalization of this old information to contemporary standards is an archaeological endeavor which was not pursued, and, thus, the reported results were taken at face value in the hope that the large sample would generally lead to a statistically-reasonable result. Where both branches of the decay were measured in the same sets of experiments, the results were combined to obtain the total (n,2n') cross sections shown in Fig. 6. The more recent results tend to have the smaller errors and to be larger at the higher energies. There have been reported three tank measurements of the total (n,2n') cross section [49 - 51]. Two of these are energy comprehensive, and are parts of large measurement programs that have proven quite reliable [49,50]. The present evaluation is based upon these tank measurements, with the results shown in Fig. 6. It is reasonable consistent with the results of the more recent activation measurements, but somewhat larger than the older activation results at energies above ≈ 16 MeV. The evaluated energy-dependent shape is qualitatively similar to the calculated predictions, but the magnitude is about 15% larger than the calculated values. Below ≈ 16 MeV, the present evaluation is similar to that given in ENDF/B-VI, as illustrated in Fig. 6. The uncertainties of the present evaluation are subjectively estimated to be ≈ 10% in regions of appreciable cross-section magnitudes. The neutron emission spectrum resulting from the scandium (n,2n') reaction was taken from vanadium evaluation of ref. [13], somewhat adjusted for the Q-values

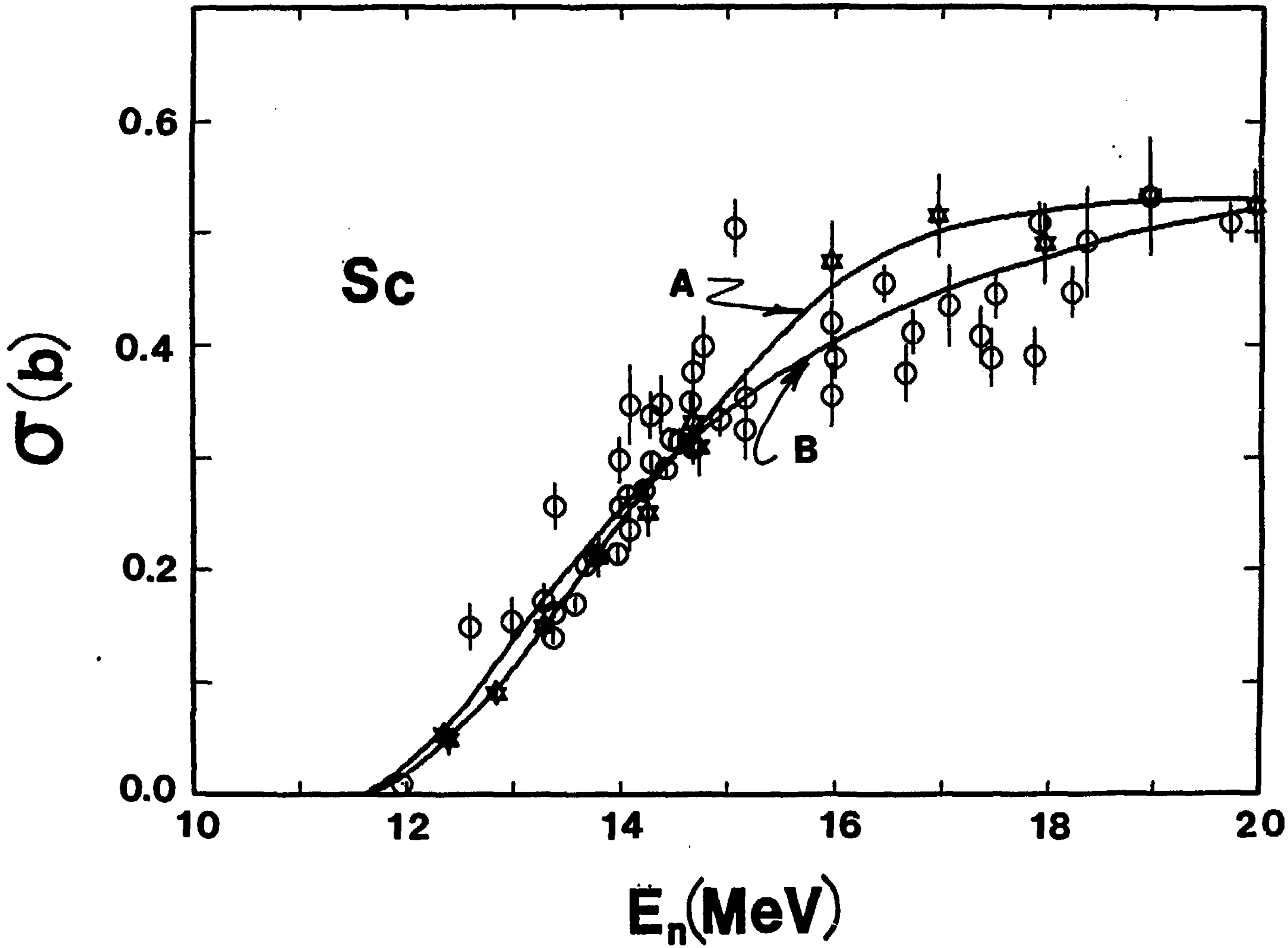

Fig. 6. Evaluated (n,2n') cross sections of scandium. Measured values obtained from activation measurements are noted by circular symbols, and those from tank measurements by "stars". Curve "A" is the present evaluation, and "B" that of ENDF/B-VI.

of the scandium reaction.

The present evaluation is not grossly uncertain. However, it is largely based on two tank measurements, and there is no technological reason why very precise results can not be obtained with contemporary activation methods and knowledge of flux standards. Therefore:-

-- Recommendation:- Both decay branches from the $^{45}Sc(n,2n')^{44}Sc^{m,g}$ reaction should be concurrently measured from threshold to ≈ 20 MeV with precisions of ≤ 3%.

Such measurements are generally within the capability of a number of modest facilities.

B. The (n,p) Reaction

There are only three differential measurements of this cross section, all activation measurements, and all grouped about 14 MeV [52 - 54]. Therefore, primary reliance had to be placed upon the model calculations. The latter results followed the general energy dependence of the measured values over their limited energy range but had to be normalized by X 0.875 to obtain the agreement with the measured results shown in Fig. 7. Away from 14 MeV, the evaluation relies entirely upon the renormalized calculations. These show a large peak at several MeV (see Fig. 7) that is attributed to the high probability of the transmission to the ^{45}Ca ground state. This is an unusual behavior, but in the absence of any experimental evidence to support or refute the calculated shape, the calculated prediction was accepted for the evaluation. Near 14 MeV the evaluation is estimated to be reliable to ≈ 10%. At other energies the values are speculative until some experimental guidance becomes available.

-- Recommendation:- Sc(n,p) activation measurements should be extended from ≈ 14 to threshold. Even qualitative results would be helpful.

Such measurements are technologically feasible. There is no (n,p) process in ENDF/B-VI for comparison.

C. The (n;n',p) and (n,d) Processes

Both of these reactions lead to stable ^{44}Ca and, therefore, are not measurable by activation methods. There appears to be no direct-particle-detection experimental information. Therefore, the evaluation relies entirely upon the calculational estimates. The neutron emission from the (n;n',p) process is approximated with a simple temperature distribution. These evaluated quantities are only

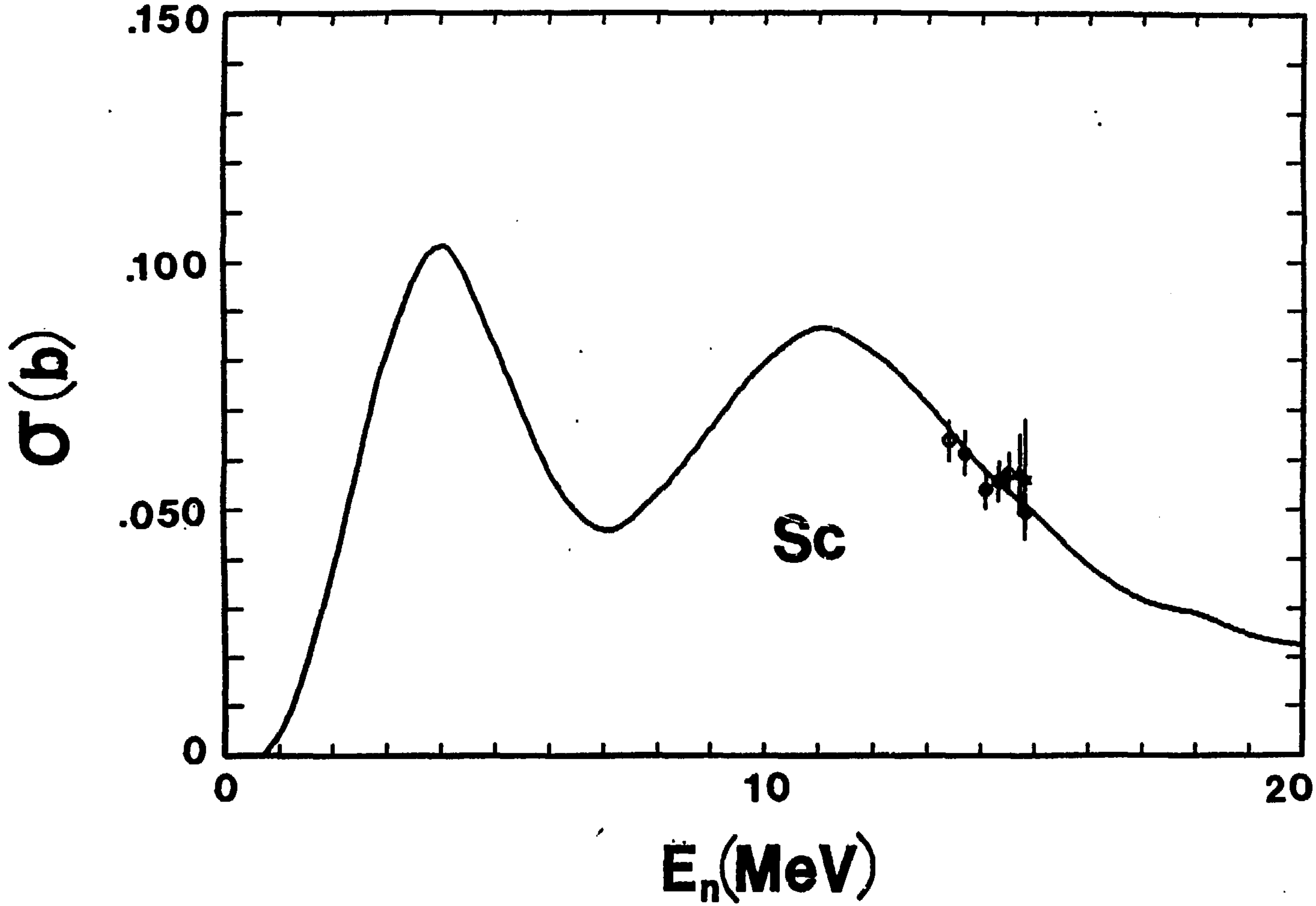

Fig. 7. Measured (symbols) and evaluated (curve) (n,p) cross sections of scandium.

qualitative. This shortcoming is not a concern in most applications as the (n;n',p) cross section is not large below 14 MeV, and the (n,d) cross section is small over the entire energy range.

-- Recommendation:- Significant improvement in the (n;n',p) and (n,d) evaluations will require some, at least, qualitative direct measurements of the the emission of the proton and the deuteron.

Such measurements are feasible but difficult. The ENDF/B-VI file contains no analogous reactions for comparison.

D. The (n,t) Process

The situation is analogous to that for the (n;n',p) and (n,d) processes, outlined above. Therefore, the same calculational approach was used to obtain a qualitative evaluation. The resulting cross sections are very small. ENDF/B-VI contains no comparable information.

E. The (n,^{3}He) Process

There are only two relevant activation measurements of this cross section [55,56], both near 15 MeV. With this fragmentary experimental information, the evaluation is based upon calculational estimates. The result is qualitative, but the cross sections are certainly very small so of little concern in most neutronic applications. There is no comparable ENDF/B-VI information.

F. The (n,α) and (n;n',α) Processes

There appear to be no relevant measurements of either of these processes. Thus, again, the evaluation relies entirely upon the calculational estimates. The neutron emission spectrum from the (n;n',α) process is represented as a simple temperature distribution. ENDF/B-VI contains no comparable information.

-- Recommendation:- It will be difficult to improve the α-emission portion of the evaluation without, at least, some qualitative experimental information.

This will probably require direct α-particle-detection measurements. These are difficult but feasible.

This Section is concluded with Fig. 8 showing the evaluated (n,p), (n;n',p), (n,α) and (n,n',α) cross sections. The remainder of

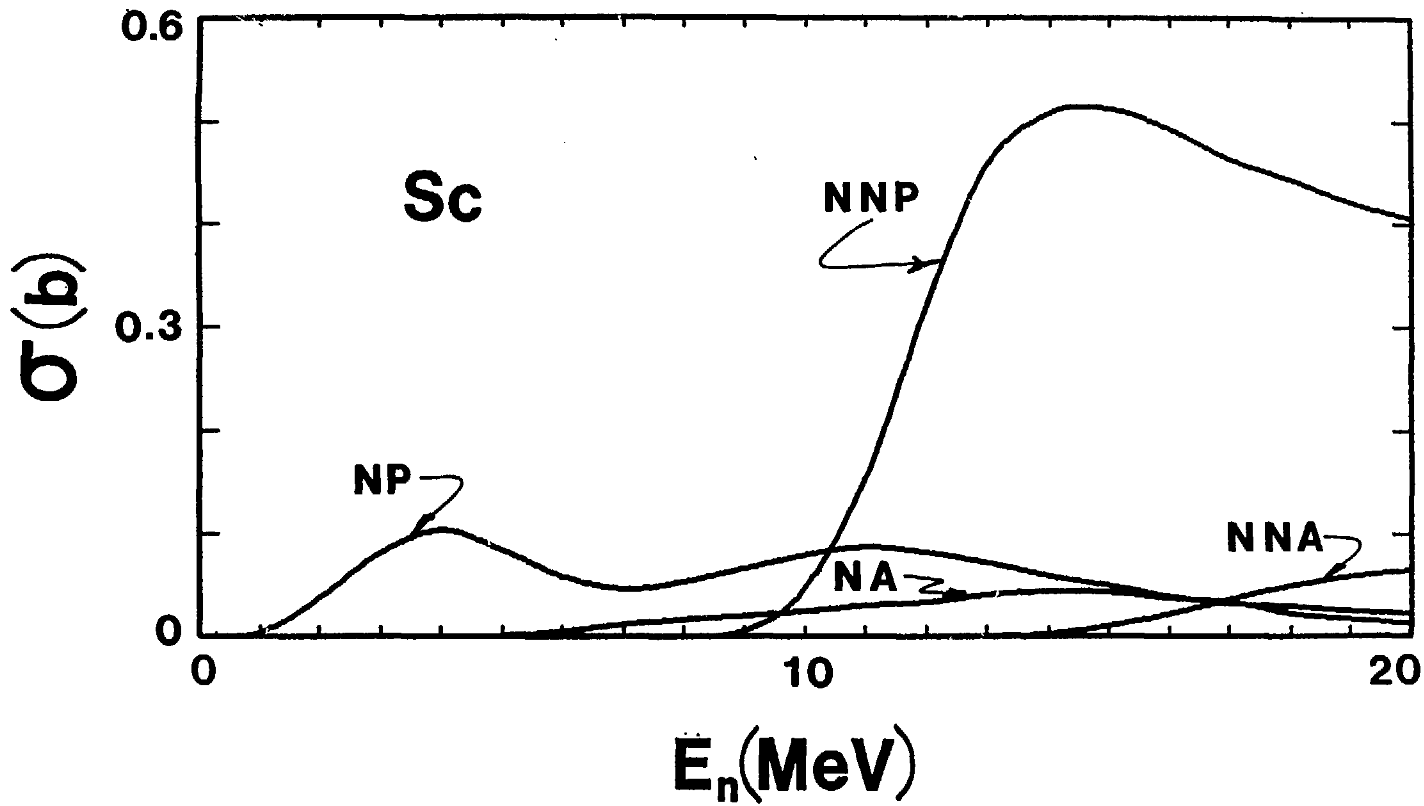

Fig. 8. Evaluated (n,p), (n;n',p), (n,α) and (n;n',α) cross sections.

the charged-particle-emitting cross sections are relatively quite small.

VII. PHOTON PRODUCTION

Photon-production data consists of contributions from (n,γ) and (n;n',γ) processes, and from a continuum of all other photon-producing reactions. Energy-dependent photon multiplicity and spectra are provided for the (n,γ) reaction. The spectrum of photons from the neutron-capture reaction was taken from the thermal-energy work of Orphan et al. [57]. The average energy of the spectrum was determined and divided by the Q-value of the reaction to obtain the low-energy photon multiplicity. The same spectrum was used at 20 MeV, with the multiplicity adjusted to conserve energy. Warren's code CASCADE [58] (which employs the method of Reffo's BRANCH code [59]) was used to obtain the energy-dependent cross sections for specific photons resulting from the de-excitation of levels excited by inelastic-neutron scattering. Photon-production cross sections and spectra for the remaining reactions were calculated using the R-parameter formalism of Perkins et al. [60]. That formalism requires formal representation of the energy distributions for all secondary particles (charged particles and neutrons) in order to calculate the photon-production and spectra. Since ENDF/B-VI formats and procedures allow for secondary charged-particle distributions in File-5 only if there is a single secondary particle, the file was translated to the ENDL format where energy distributions for all secondary particles can be represented. The necessary R(U) values were obtained from the work of Newman and Morgan [61] since the scandium mass is at the lower extreme of the "global" R(U) values used for heavier elements.

VIII. SUMMARY REMARKS

This work provides a comprehensive scandium evaluated data file for neutronic calculations where none previously existed. The file content is as precise as reasonably possible given the sparse experimental data base for the neutron interaction with scandium. Significant improvements will require extensive measurements as outlined in the following recommendations. Many of these measurements involve monoenergetic neutron sources.

-- Recommendation:- Re-interpret the resonance region of scandium making use of the most recent experimental data sets.

-- Recommendation:- Measure energy-averaged scandium neutron total cross sections from 0.1 to 20 MeV with accuracies of $\leq$ 2%. At the lower extreme of this energy range, attention must be given to self-shielding effects and resonance structure. Such measurements are technologically feasible.

-- Recommendation:- Several good-quality differential elastic scattering measurements are needed between ≈ 10 and 20 MeV to confirm the energy behavior of the model used in the evaluation. Such measurements are technologically feasible.

-- Recommendation:- Several double-differential neutron scattering measurements are needed, distributed over incident energies of 5 - 20 MeV, to define the evaluated continuum inelastic-neutron spectra. Such measurements are notoriously difficult above ≈ 10 MeV.

-- Recommendation:- The Sc(n,γ) cross section should be measured with broad incident-neutron resolution from ≈ 100 keV to several MeV. The measurements will be tedious but are technically feasible, and accuracies of even 25% would be very useful.

-- Recommendation:- Both decay branches from the ^{45}Sc(n,2n')^{44}Sc^{m,g} reaction should be concurrently measured from threshold to ≈ 20 MeV with precisions of $\leq$ 3%.

-- Recommendation:- Sc(n,p) activation measurements should be extended from ≈ 14 to threshold. Even qualitative results would be helpful.

-- Recommendation:- Significant improvement in the (n;n',p) and (n,d) evaluations will require some, at least, qualitative direct measurements of the the emission of the proton and the deuteron.

-- Recommendation:- It will be difficult to improve the α-emission portion of the evaluation without, at least, some qualitative experimental information.

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