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NEUTRON CROSS SECTIONS AND THEIR UNCERTAINTIES OBTAINED FROM NUCLEAR SYSTEMATICS*

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Previously, neutron cross sections in the MeV range for nuclei ranging in Z from 21 through 41 were calculated using a hybrid empirical-statistical model code THRESH. The formalism includes level density, Coulomb barrier, and competing reaction effects and has been useful in the prediction of unmeasured cross sections or normalized to point measurements to generate complete excitation curves. Reaction data up to 20 MeV in the Z range 21 through 83 are used to refine the model and extend its range of validity. A least squares fitting technique optimizes the choice of parameters with the resulting matrix used to determine parameter uncertainties and correlations. Fitted cross sections and their calculated uncertainties are compared with measurements and quoted errors. A range of uncertainty is assigned to predicted cross sections.

(Neutrons; cross section; nuclear model)

Introduction

Nuclear models can be used to provide physical insight to nuclear reaction mechanisms and to supplement experimental information that is either incomplete or discrepant while also yielding data in continuous form. The nuclear model parameters can be adjusted so that the calculations agree with good experimental data thereby extending the validity of the model but due to the spread of experimental data the nuclear model results will also have a range of uncertainty. The nuclear model code THRESH[1] has been improved and used to fit (n,2n), (n,p), and (n,α) data in the nuclear charge range 21 through 83.

The THRESH code calculates (n,particle) reactions in the MeV range using a hybrid empirical-statistical model but the results are not expected to be accurate in detail. No discrete level information is used and de-excitation of the compound nucleus by photon emission is ignored. Approximate formulas for components of the reaction mechanism are employed. In fact, only Z and A of the target nucleus is required as input although the calculated binding energies and any of 13 stored parameters may be overridden by the user if desired. The code has been very useful in evaluations of neutron cross sections for primary and secondary particle emission in the energy range to 20 MeV mainly because of the scarcity of experimental data and the detailed information required as input by other nuclear model codes.

Cross Section Systematics

The 14 MeV cross sections appear to vary in a systematic way with the neutron asymmetry parameter

$$s = \frac{N-Z}{N+Z} . \tag{1}$$

The (n,2n) reaction has been studied by several authors[2,3,4,5] with the premise that the channel for emitting neutrons $\sigma_{n,N}$ is in ratio to the nonelastic cross section σ_{ne} according to the following formula

$$\frac{\sigma_{n,N}}{\sigma_{ne}} = 1 - \alpha_N e^{-\beta_N s} \tag{2}$$

It is therefore not surprising that the remainder of the nonelastic cross section channels leading to charged particle emission are expected to vary exponentially with s according to

$$\frac{\sigma_{n,p}}{\sigma_{ne}} = \alpha_p e^{-\beta_p s} \quad \text{and} \tag{3}$$

$$\frac{\sigma_{n,A}}{\sigma_{ne}} = \alpha_A e^{-\beta_A s} \tag{4}$$

for (n,p) and (n,α) reactions respectively. Several authors[6,7,8,9] have proposed exponential formulas for the (n,p) and (n,α) cross sections at 14 MeV as described in Table I. There are significant differences among the proposed formulae that suggest it would be difficult to describe 14 MeV cross sections for emitting charged particles by a simple exponential formula.

Typical (n,p) cross section excitation curves are shown schematically as a function of energy and s in Figure 1. For small s, tending to describe a light nucleus with a small Coulomb barrier, (n,p) cross section has already peaked below 14 MeV and is decreasing due to competing reactions that are energetically possible. At intermediate values of s, for the cross section peak occurs at about 14 MeV. For large values of s, indicating a heavy nucleus with a high Coulomb barrier, the 14 MeV cross section occurs between threshold and the peak and is strongly dependent on barrier penetration characteristics. Thus 14 MeV cross sections sample widely different reaction phenomena and do not lend themselves to a few parameter fit. On the other hand the magnitude of the reaction channel which is approached by the peak cross section appears to vary systematically with s which serves as a simple indicator of a competion between neutron and charged particle emission.

Fitting Procedure

The cross section at energy E_n can be calculated using a nuclear model code with M parameters P_m

$$\sigma_n(E) = f\,(P_1, P_2 \text{----} P_M,\ E_n) \tag{5}$$

Denoting chi-square for N data points D_n of weight W_n as

$$\chi^2 = \sum_{n=1}^{N} W_n\,(D_n - \sigma_n) \tag{6}$$

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and creating a Taylor expansion about σ^0, determined from an initial set of parameter guesses, leads to the following minimization of χ^2 with respect to P_k

$$\sum_{n=1}^{N} W_n \sum_{m=1}^{M} \frac{\partial\sigma_n}{\partial P_m} \frac{\partial\sigma_n}{\partial P_k} \, dP_m = \sum_{n=1}^{N} W_n (D_n - \sigma_n^o) \frac{\partial\sigma_n}{\partial P_k} \qquad (7)$$

Equation 7 represents the normal equations to be solved simultaneously for a least squares fitting of the data. The matrix equation of the form

$$A \cdot dP = B \qquad (8)$$

is solved by inverting the A matrix to yield the column matrix dP, whose elements are the increments to the trial parameters P.

$$P_k^1 = P_k^0 + dP_k \qquad (9)$$

The process is repeated with the help of acceleration techniques until the solution has converged.

The uncertainties in the cross sections are expressed by the following equation.

$$d\sigma_n^2 = \sum_{k=1}^{M} \sum_{\ell=1}^{M} \left(\frac{\partial\sigma_n}{\partial P_k}\right)\left(\frac{\partial\sigma_n}{\partial P_\ell}\right) \langle dP_k \cdot dP_\ell \rangle \qquad (10)$$

where

$$\langle dP_k \cdot dP_\ell \rangle = A_{k\ell}^{-1} \frac{\chi^2}{N-M} \qquad (11)$$

and the correlation $C_{k\ell}$ between parameters dP_k and dP_ℓ is

$$C_{k\ell} = \frac{\langle dP_k \cdot dP_\ell \rangle}{dP_k \cdot dP_\ell} \le 1 \qquad (12)$$

For 14 MeV (n,2n) data an evaluation[10] consisting of 98 nuclides and for (n,p) data a 132 nuclide evaluation[11] were used for fitting. For 14 MeV (n,α) data the experimental results of several authors[7,9,12,13,14,15] consisting of 90 data points for 66 nuclides was used. Energy dependent data for several nuclides were taken from the ENDF/B-IV library for cases where it could be ascertained that the evaluations were based on measured data.

Results

The range of uncertainties indicated by equation 10 is shown in Table II. Included is the estimated 10% uncertainty in the nonelastic cross section. In 30 to 50 percent of the cases the measured data lie outside the range of its fitted cross section and estimated uncertainty. For heavy nuclides the (n,2n) cross section approaches the nonelastic cross section whose error dominates the uncertainty the (n,p) and (n,α) cross sections are small and often highly uncertain.

The results of using the generalized parameters obtained from the least squares fitting of experimental data to fit the ^{56}Fe (n,p) cross section is shown in Figure 2. The ENDF/B-IV data are based on measurements. The agreement between calculation and experiment is improved by particularizing the parameters to the ^{56}Fe (n,p) cross section. However, the calculation does not agree near threshold due to deficiencies of the model in the calculation of threshold effects and excitation of particular states.

Some specific cases for the (n,α) reaction are shown in Table III. The two measurements for the ^{51}V (n,α) cross sections differ by a factor of 2 1/2 despite the assignment of small uncertainties. The results of the adjusted THRESH calculations have a ±5% uncertainty but support the measurement of Levkowski[9]. For similar reasons the Sato[14] results are preferred over the measurements of other authors for ^{68}Zn, ^{79}Br, and ^{81}Br. These are a few examples of how the uncertainties in the cross sections obtained from nuclear model fitting of experimental data can be helpful in the selection of preferred values from among discrepant measurements.

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Table I

<u>14 MEV SYSTEMATICS</u>

$\frac{\sigma_{n,p}}{\sigma_{ne}} = ke^{-25.2\frac{N-Z}{N+Z}}$, $\frac{\sigma_{n,\alpha}}{\sigma_{ne}} = ke^{-31.1\frac{N-Z}{N+Z}}$	Bayhurst	1961
$\sigma_{n,p} = 0.60\,(N-Z)^2 e^{-62.8\frac{N-Z}{N+Z}}$, $\sigma_{n,\alpha} = 0.70e^{-28\frac{N-Z+1}{N+Z}}$	Havlik	1971
$\sigma_{n,\alpha} = 45.2\,(A^{\frac{1}{3}}+1)^2 e^{-65\frac{N-Z-L}{N+Z-L}}$	Choudhury	1971
$\frac{\sigma_{n,p}}{\sigma_{ne}} = 0.73e^{-33\frac{N-Z}{N+Z}}$, $\frac{\sigma_{n,\alpha}}{\sigma_{ne}} = 0.29e^{-33\frac{N-Z}{N+Z}}$	Levkovski	1971

Table II

<u>RANGE OF UNCERTAINTIES (%)</u>

Reaction	$\frac{N-Z}{N+Z}$ .03-.05	.05-.10	.10-.15	.15-.20
n,2n	20-50	10	10	10
n,p	20-25	20-30	20-40	30-150
n,α	25	25-40	30-60	40-150

Table III

<u>EXAMPLES OF FITTED AND MEASURED RESULTS</u>

Reaction	THRESH	Measurements		
$^{51}V\,(n,\alpha)$	18 ± 5	43 ± 4	Chatterjee	1963
		18 ± 3	Levkowski	1971
$^{68}Zn\,(n,\alpha)$	6.6 ± 1.8	15 ± 2.5	Qusim	1971
		8 ± 0.5	Sato	1971
		9 ± 1	Levkowski	1971
$^{79}Br\,(n,\alpha)$	8 ± 2	20 ± 2	Venugopala	1971
		10.8 ± 0.7	Sato	1971
		15 ± 3	Levkowski	1971
$^{81}Br\,(n,\alpha)$	3.6 ± 1.4	19 ± 2	Venugopala	1971
		3.7 ± 0.3	Sato	1971
		7 ± 1	Levkowski	1971

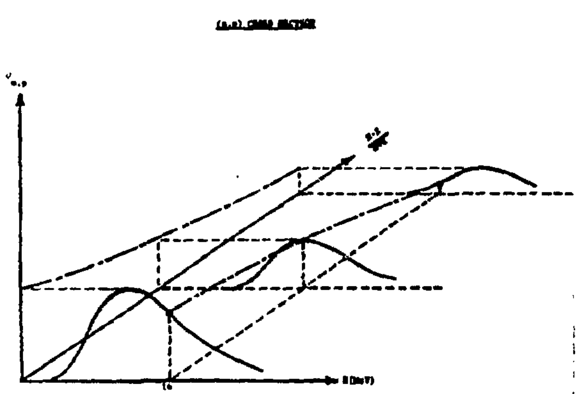

Figure 1

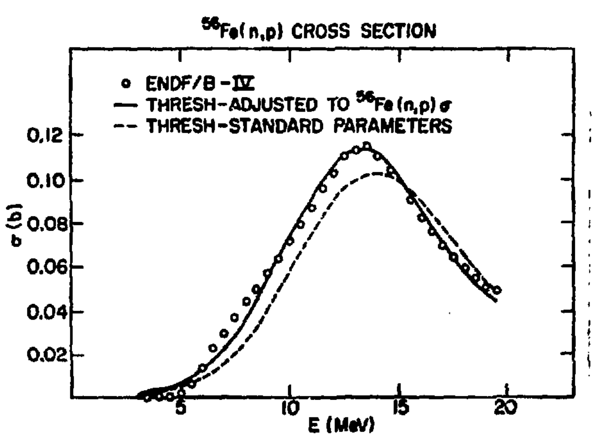

Figure 2

41