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Report to the ^{238}U Discrepancy Task Force on SIOB Fits to the ORNL, CBNM, and JAERI Transmission Data

D. K. Olsen

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ABSTRACT

The computer code SIOB has been used to obtain least-squares simultaneous-sample shape fits to the recent ^{238}U transmission data of ORNL, CBNM, and JAERI over the energy regions 1460 to 1820 eV, 2470 to 2740 eV, and 3820 to 4000 eV. The fits indicate that much of the systematic discrepancy in the published neutron widths from these data arose in the data analysis procedure. Except for the 3820- to 4000-eV JAERI data, the systematic differences in the resulting neutron widths from the present analyses of the three measurements with no background corrections is less than 2 to 4%. The neutron widths are larger than those contained in any existing evaluation. These fits were performed as part of the work for the NEANDC ad hoc ^{238}U Discrepancy Task Force.

1. INTRODUCTION

Least-squares shape fits to three energy regions each of the recent Oak Ridge National Laboratory (ORNL),[1,2] Central Bureau for Nuclear Measurements (CBNM),[3] and Japan Atomic Energy Research Institute (JAERI)[4] ^{238}U transmission data have been performed using the ORNL computer code SIOB.[2,5] The purpose of this work was to determine whether the apparent systematic discrepancies in the published neutron widths from these data are caused by systematic differences in the reduced transmission data or whether the neutron-width discrepancies are introduced in the data analyses procedures. These calculations were done in response to the work of the Nuclear Energy Agency Nuclear Data Committee (NEANDC) ad hoc task force on discrepancies in ^{238}U differential data.

Figure 1 shows the neutron-width discrepancy in terms of average strength functions over 0.5-keV intervals. On a resonance-by-resonance basis the systematic discrepancies are larger than those shown in Fig. 1. The recent ENDF/B-V evaluation[8] gives a systematic uncertainty in the neutron widths which increases linearly from 4% at low energies to 20% at 4 keV. The resolved-resonance neutron widths seem to need to be known to about 3 to 5%. From this work it is found that many of the systematic discrepancies in the published neutron widths were introduced in the data analyses procedures. Except for the JAERI data,[4] at high energies where there probably exists a background subtraction error, the systematic differences in the neutron widths from SIOB analyses of the three measurements with no background corrections are less than 2 to 4%. The major points from this work are listed in the summary.

The three data sets were fit with SIOB over the following energy regions: Region 1, 3820 to 4000 eV; Region 2, 2470 to 2749 eV; and Region 3, 1460 to 1820 eV. These energy regions are shown in Figs. 2 through 5 with the CBNM data[3] for transmission through their 0.035-b^{-1} sample. Figures 6, 7, and 8 show the three data sets over the 3858-eV and 3873-eV resonances. The approximate contributions to the total resolution at 4 keV, excluding exponential tails, are listed in Figs. 6 to 8. Details of the measurements are given in refs. 1 to 4 and listed in Table 1. Only the JAERI transmission[4] data for the cooled sample measured with 62.5-ns-wide bursts have been analyzed in this report.

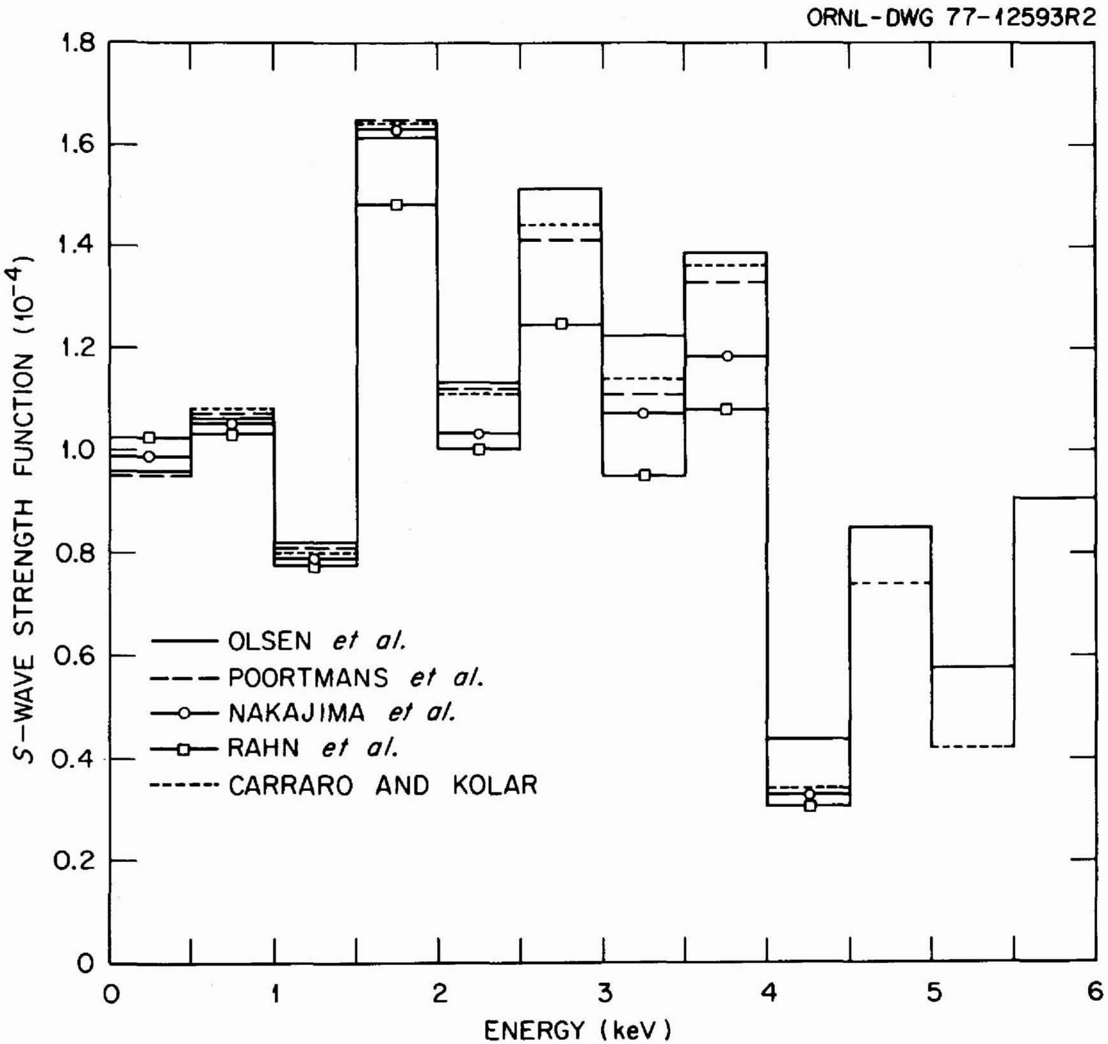

Fig. 1. Comparison of local s-wave strength functions of ^{238}U for 0.5-keV intervals from ORNL (refs. 1 and 2), CBNM (ref. 3), JAERI (ref. 4), Rahn et al. (ref. 6), and Carraro and Kolar (ref. 7). Each interval contains about 20 resonances.

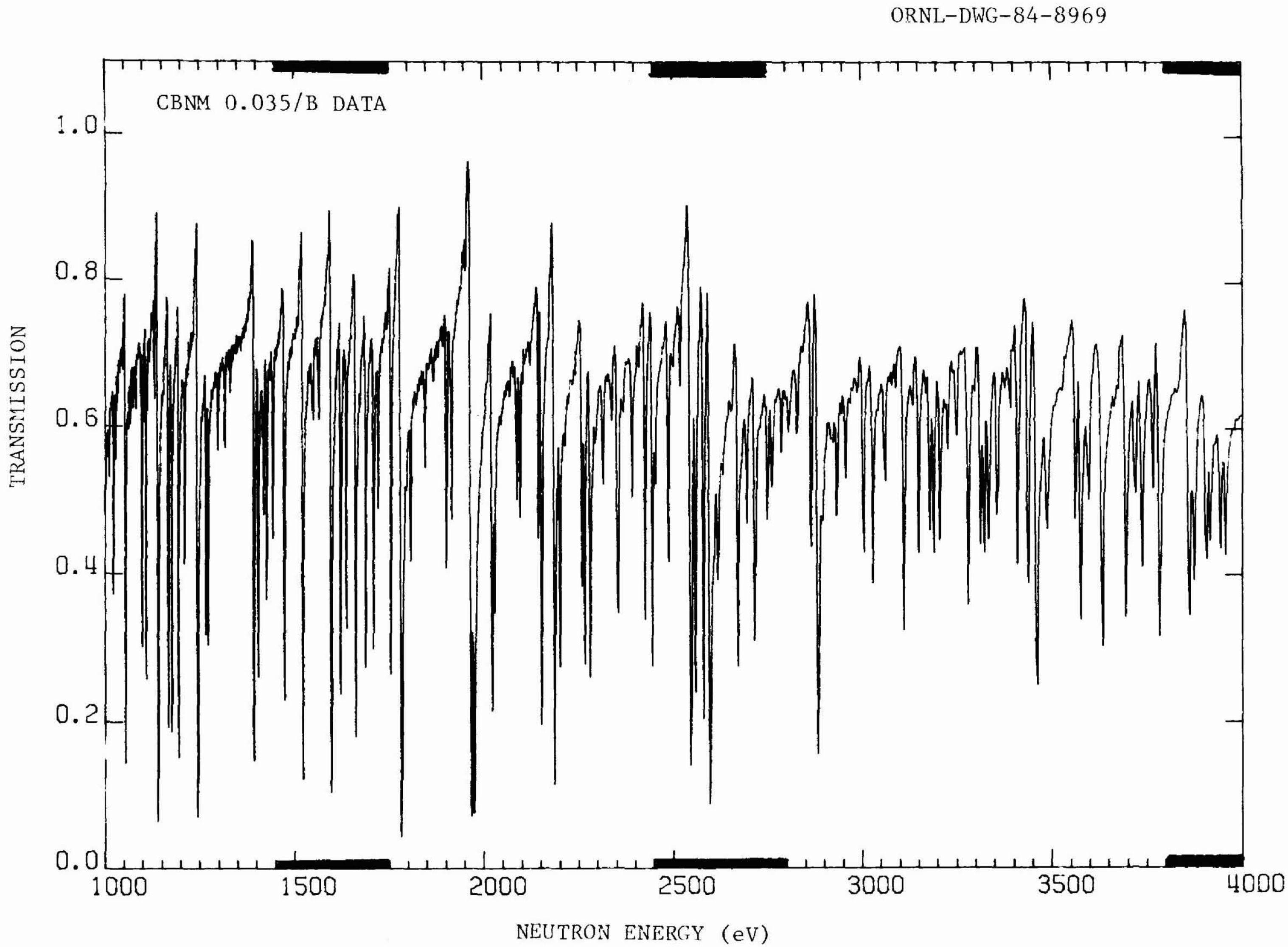

Fig. 2. Measured transmission (ref. 3) through a 0.035 b^{-1} ^{238}U sample. The heavy parts of the energy scale shows the regions fitted in this study.

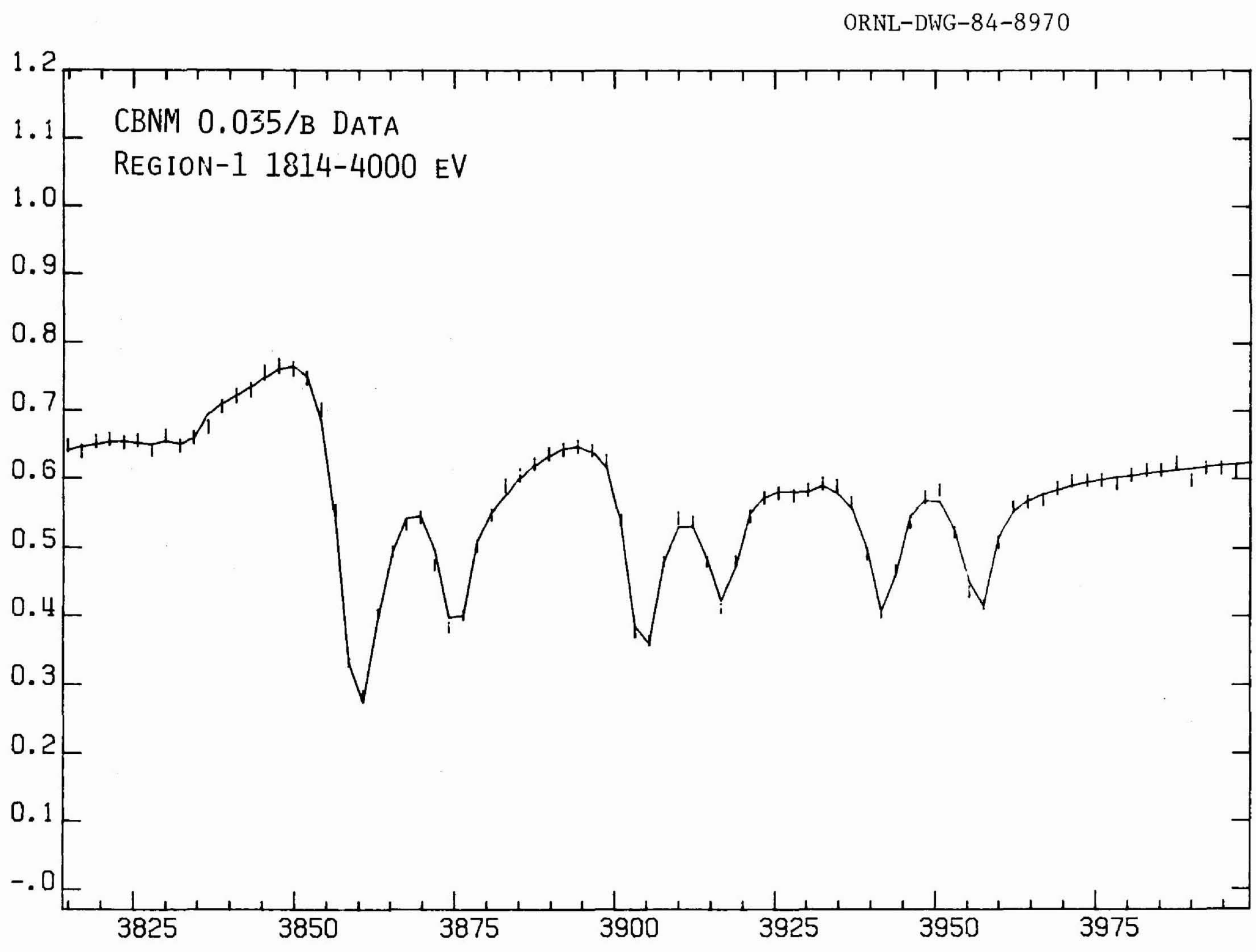

Fig. 3. Measured transmission (ref. 3) through a 0.035 b^{-1} ^{238}U sample over energy region 1 which contains six large s-wave resonances.

ORNL-DWG-84-8971

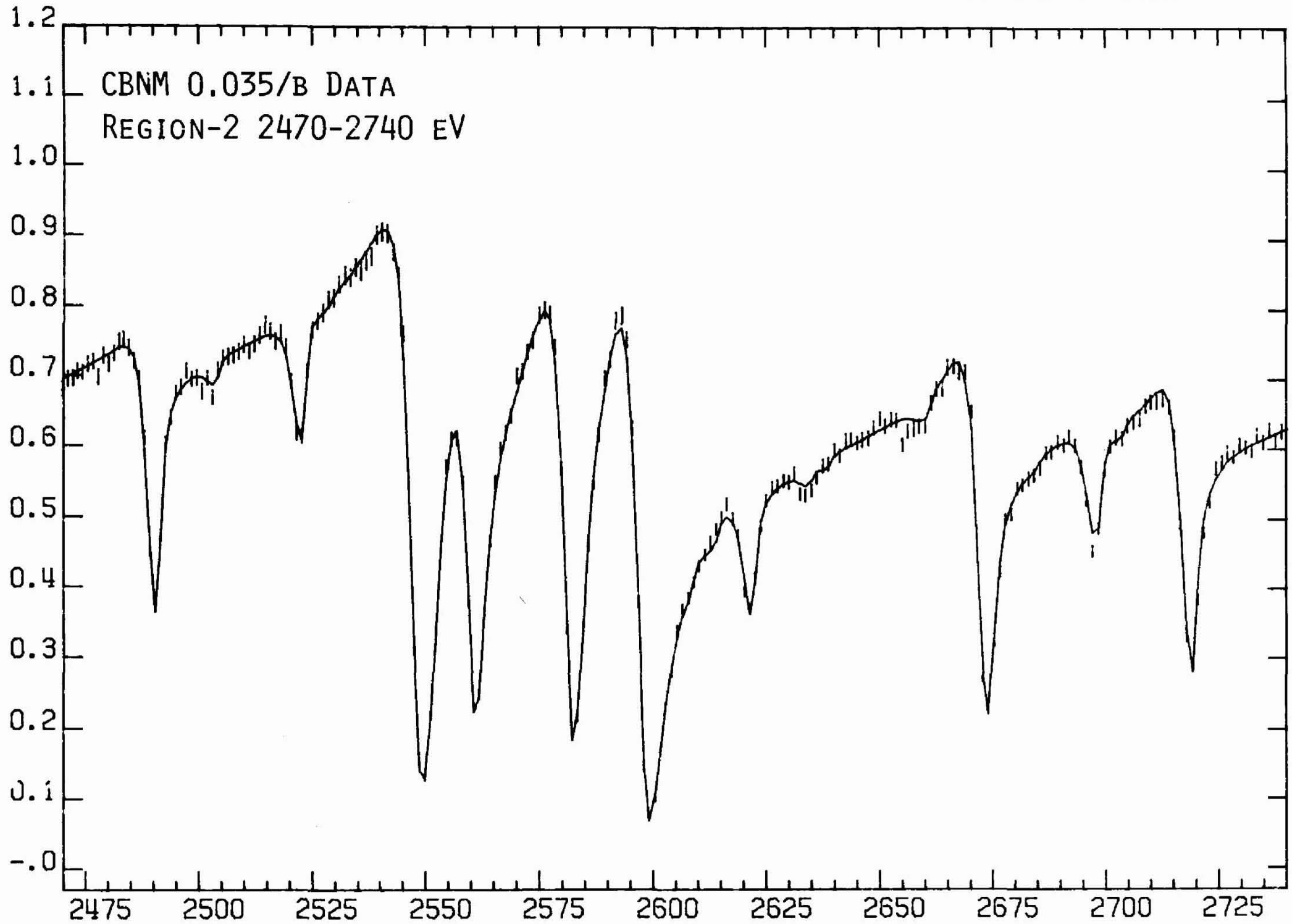

Fig. 4. Measured transmission (ref. 3) through a 0.035 b^{-1} ^{238}U sample over energy region 2 which contains ten large s-wave resonances.

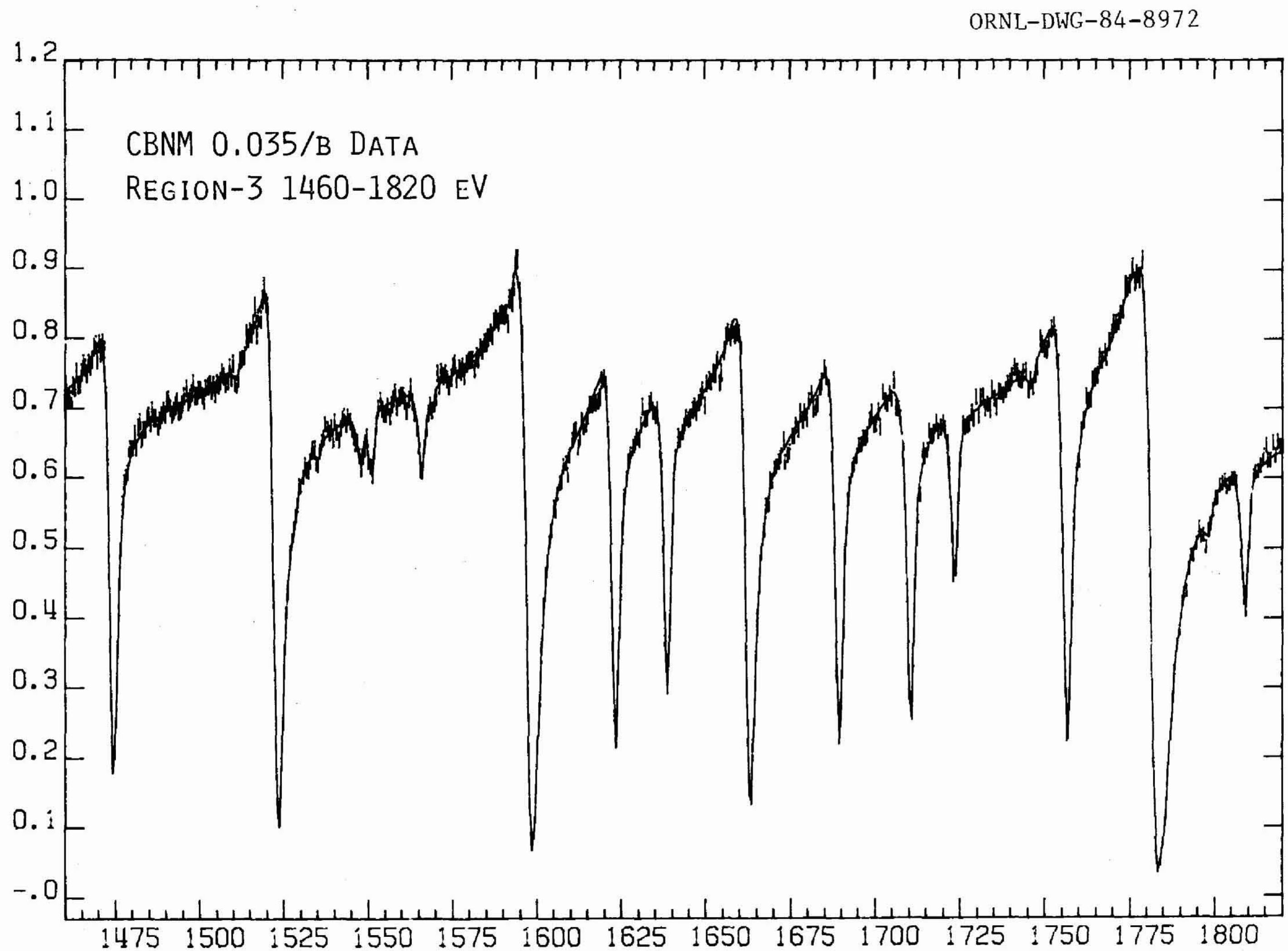

Fig. 5. Measured transmission (ref. 3) through a 0.035 b^{-1} ^{238}U sample over energy region 3 which contains 12 large s-wave resonances.

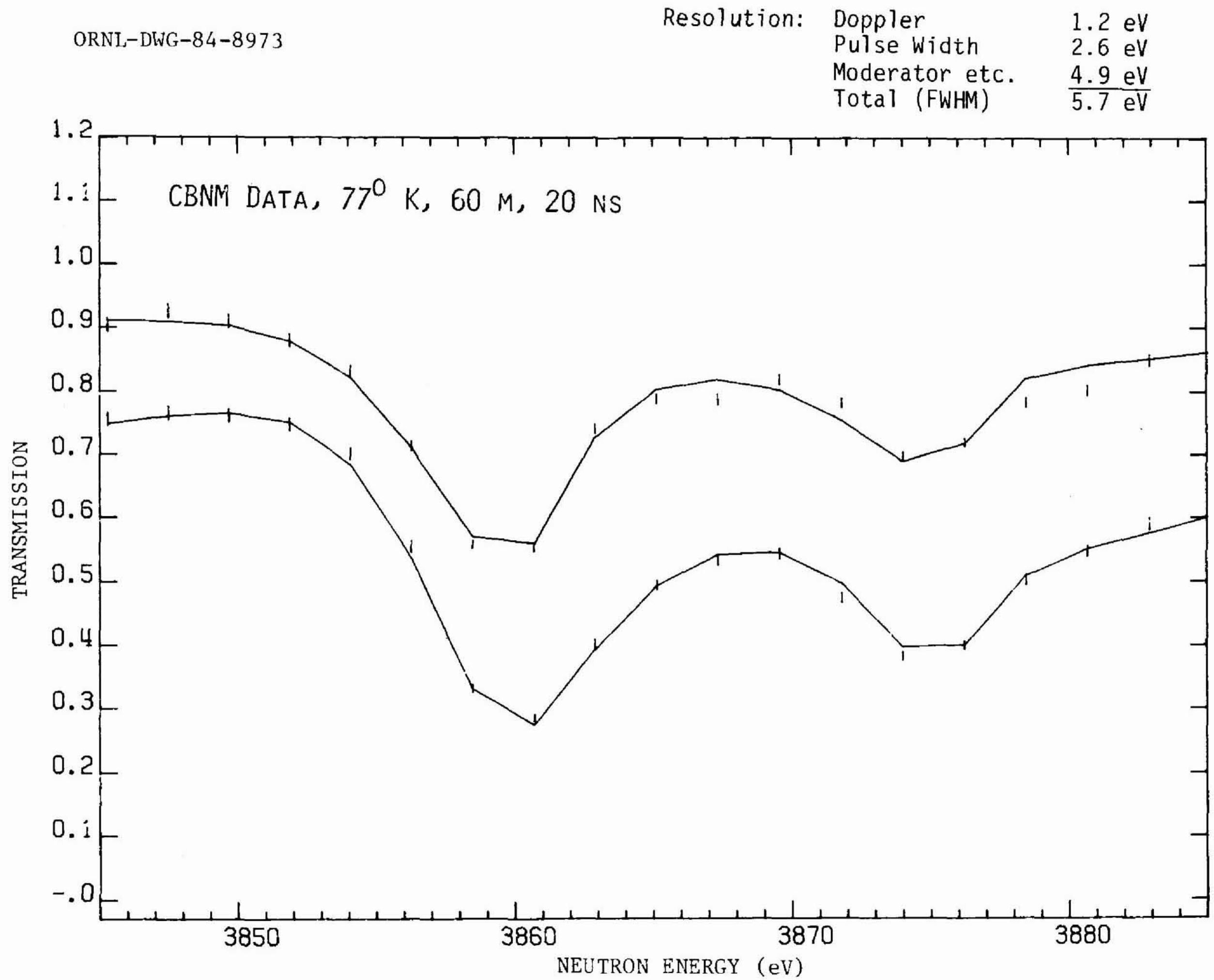

Fig. 6. Least-squares fit to the CBNM data (ref. 3) over the 3858- and 3873-eV resonances. The total resolution is 5.7 eV.

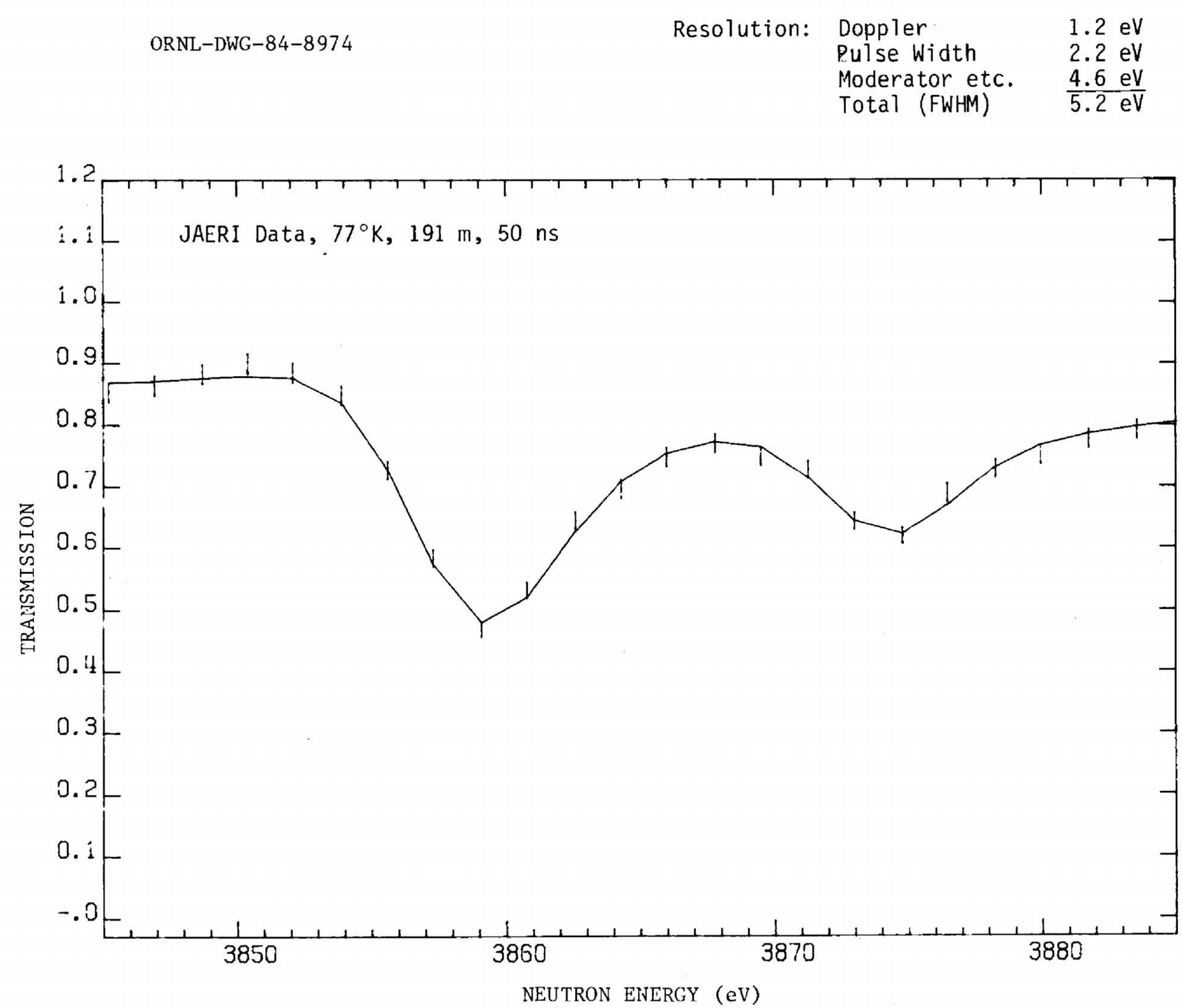

Fig. 7. Least-squares fit to the JAERI data (ref. 4) over the 3858- and 3873-eV resonances. The total resolution is 5.2 eV.

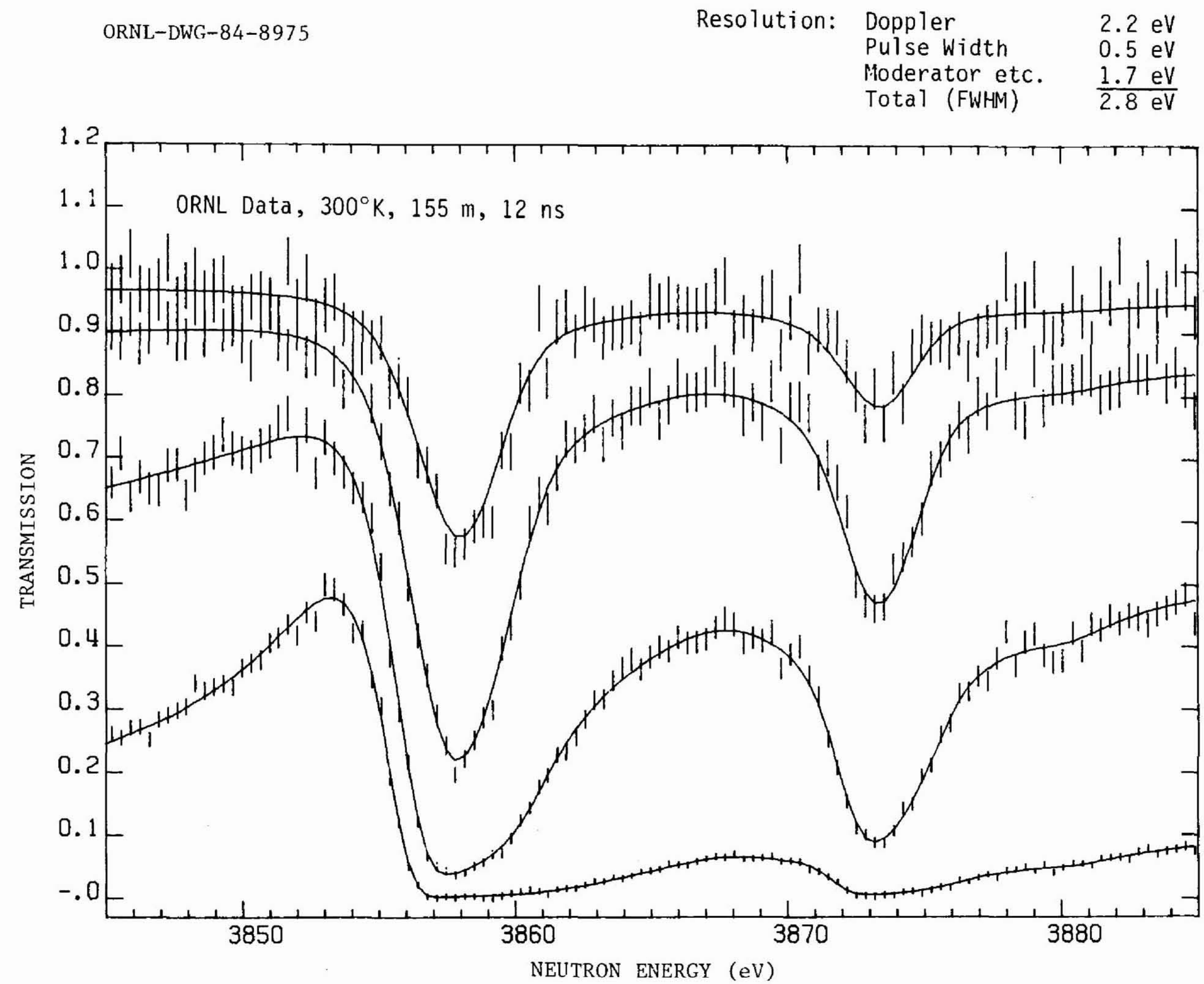

Fig. 8. Least-squares fit to the ORNL data (refs. 1 and 2) over the 3858- and 3873-eV resonances. The total resolution is 2.8 eV.

Table 1. Measurement details

	ORNL	CBNM	JAERI
Sample thickness (b^{-1})	0.175		
	0.052	0.035	
	0.012	0.010	0.014
	0.004		
Sample temperature (°K)	300	77	77
Flight path (m)	155	60	191
Burst width (ns)	12	23	62.5
Detector	12-mm Li-glass	^{3}He gas	Li-glass array
Equivalent resolution distance (mm)	35	38	110
Subtracted background	2.5%	4%	?

2. THE SIOB RESOLUTION FUNCTION

Table 2 gives a precise definition of the resolution function employed in SIOB for this study. This resolution function was initially chosen to fit the ORNL 150-m ^{238}U transmission data. The SIOB resolution function consists of a convolution of a moderator (or Gaussian) function with an exponential-tail function. The most important resolution component is the time response of the target-moderator at the Oak Ridge Electron Linear Accelerator (ORELA). This has been Monte Carlo calculated[9] and is plotted as histograms in terms of equivalent distance in Fig. 9. These histograms have been fitted with functions of the form $x^n e^{-x}$. These are the mathematical forms used for the SIOB moderator function. The SIOB parameter d is the FWHM of these distributions in mm, excluding the burst time width. In the keV region the Monte Carlo calculations[9] give a d of around 24 mm. The form x^2e^{-x} has been used for the present study; however, the forms x^3e^{-x}, x^4e^{-x}, and x^5e^{-x} would probably give the same results. Note also, as shown in Table 2, that the burst time width is included with the form x^2e^{-x} but its contribution to the width is not included in d. All other resolution effects except an exponential tail must be accounted for with d. SIOB also has the option to use a Gaussian function. For either option, d has the same physical meaning.

The second most important contribution to the resolution function of the ORNL data is the multiple scattering in the 12-mm-thick Li-glass scintillator and 13-mm-thick quartz light pipe used as a neutron detector. Figure 10 shows a Monte Carlo calculation[10] of the time response of this detector for 3.3-keV neutrons. About two-thirds of the (n,α) events are prompt and about one-third of the (n,α) events occur after some initial scattering. These multiple-scattering events give rise to an exponential tail as shown. The SIOB exponential-tail function is parameterized in terms of L (equivalent-distance half-life in mm) and F (the fraction in the exponential tail). These variables can be least-squares fitted to the transmission data. Monte Carlo calculations[10] of the time response of ORELA detector from about 1 to 10 keV give L and F to be 20 mm and 0.35, respectively, independent of neutron energy. Note that the detector thickness must be accounted for with d since the $(1\text{-}F)$ piece is folded with a delta function.

Table 2

NORMALIZED MODERATOR FUNCTIONS

Option 1: $\exp(-x^2)/\sqrt{\pi}$, $-\infty < x < \infty$, mean = 0, FWHM = 1.665

$$T'(E) = \int_{-\infty}^{+\infty} \exp[-(E-E')^2/\epsilon^2]T(E')dE'/(\sqrt{\pi}\epsilon)$$

Option 2: $x^2 \exp(-x)/2$, $0 < x < \infty$, mean = 3, FWHM = 3.394

$$T'(E) = \int_{E-3\epsilon}^{\infty} [3+(E-E')/\epsilon]^2 \exp(-3-(E-E')/\epsilon]T(E')dE'/(2\epsilon)$$

where $\epsilon = E(\text{eV})\sqrt{b+c\cdot E(\text{eV})}$

$b = (2/\text{FWHM})^2\,[d(\text{fwhm-mm})/\text{FPL(mm)}]^2$

$c = (2/\text{FWHM}/72.3)^2\,[\Delta t(\text{fwhm-ns})/\text{FPL(mm)}]^2$

b and c can be varied. Usually b is varied and c is calculated and fixed.

NORMALIZED EXPONENTIAL TAIL FUNCTION

$$T''(t) = (1-F)T'(t) + F\int_0^t \exp[-\lambda(t-t')]T'(t')\lambda dt'$$

where $\lambda(1/\text{ns}) = (0.6931/72.3)\sqrt{E(\text{eV})}\,/L(\text{mm})$.

L and F can be varied. L is the equivalent-distance half-life of the exponential decay in mm.

SIOB BACKGROUND AND NORMALIZATION CORRECTIONS

$$T''' = (1 + N)(1 - B/T_p)\,T''(E) + B$$

N and B can be varied and act on the calculated, not measured, transmission. B is defined so that a non-zero B does not change the potential scattering transmission (T_p). Note also that B measures excess background with respect to a transmission of unity.

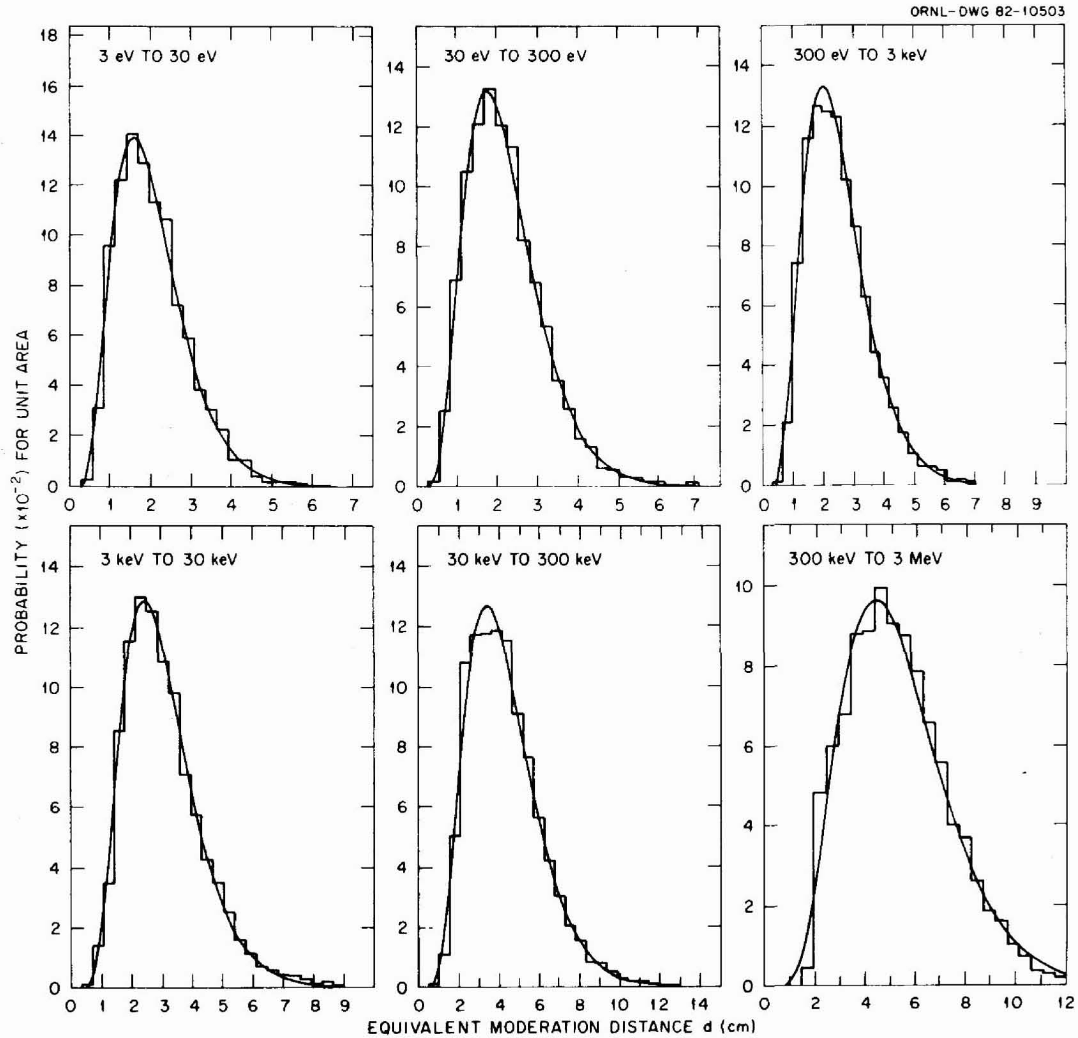

Fig. 9. Monte Carlo calculation (ref. 9) of the delay-time distribution in terms of equivalent distance from the "shadowed" ORELA target moderator. The smooth curves are fits to the distributions with functions of the form $x^n e^{-x}$.

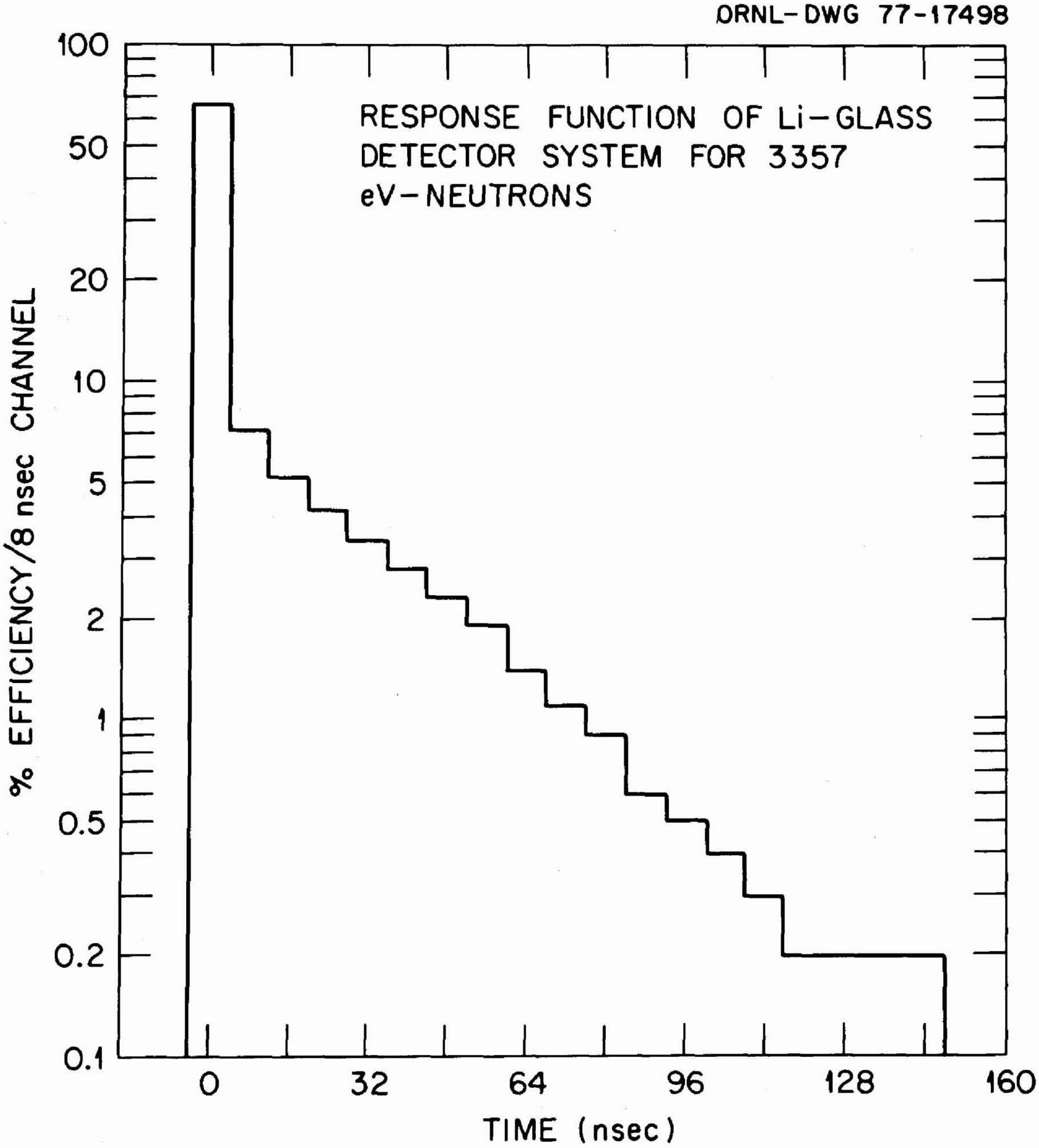

Fig. 10. Monte Carlo calculation (ref. 10) of the time response of a 12.5-mm-thick Li-glass detector illuminated with 3.4-keV neutrons.

3. SIOB COMPUTER CODE

The multi-level Breit-Wigner cross-section equations and picket-fence terms used in SIOB are given in refs. 2 and 5. The excess background and normalization correction factors and resolution functions used in this study are given in Table 2. It is important to note that the excess-background correction term in Table 2 is specifically defined so that it does not change the normalization. This allows possible errors in the subtracted background to be studied independently of the normalization and is consistent with the raw data reduction procedures used with the ORNL transmission data. SIOB is a conventional least-squares code and no uncertainties can be input except the uncorrelated statistical errors of the transmission data. Some of the procedures used for the fits are listed below:

1. A minimum statistical uncertainty of ± 0.004 was set on all input transmission data. This was initially done for the ORNL data to negate some of the heavy weight given to the thickest sample and to negate some of the very statistically-accurate data points at the bottom of black resonances which are dominated by systematic background problems. This, of course, artifically reduces the chi-square per degree of freedom, χ^2. However, it is important to appreciate that the SIOB output covariance matrix is renormalized by multiplication with χ^2 so the input statistical uncertainties on the data points act only as weights and in an absolute sense do not affect the output parameter uncertainties. The absolute value of χ^2 is somewhat meaningless anyway since, in a strict statistical sense, the χ^2 to a fit with a few thousand data points must lie between 0.999 and 1.001; this never occurs.

2. The four samples of the ORNL data were fit simultaneously, as were the two samples of the CBNM data.

3. Large resonances, ~200 eV above and below the fitted region, were explicitly contained in the cross section formula using the ORNL resonance parameters. These parameters were not adjusted. Effects from more distance resonances were included with picket-fence terms using average resonance parameters. In addition, a term of the form S log[(EH-E)/(E-EL)] was added to the cross section to account for a possible imbalance in the distant levels. For all fits S was a fitting variable. With both S and the effective radius R variable, the resonances outside the fitted region have almost no influence on the neutron widths inside the fitted region; only S and R are changed.

4. All the resonances observed in the ORNL transmission data were included in the cross sections as s-wave resonances for all fits. The parameters of the small resonances were fixed at the ORNL values for analysis of CBNM and JAERI data, so each data set was fit by an identical set of resonances.

5. For each fit the resonance energies and neutron widths were varied, as well as R and S. All capture widths were fixed at 23.5 meV.

6. For each fit the parameter c (time-width dependence) of the resolution function was calculated and fixed. The parameter b (distance-width dependence) was always a fitting variable and is given in terms of d. The parameter F was always a fitting variable and the parameter L was fixed or varied depending on the data set and energy.

7. The cross sections were Doppler broadened with a Gaussian convolution using chi and psi functions with an effective-temperature input.

4. RESOLUTION FUNCTION STUDY WITH NO EXCESS BACKGROUND AND NORMALIZATION CORRECTIONS

Table 3 lists results of fits to the three data sets over the three energy regions using four different resolution-function forms: exp($-x^2$), exp($-x^2$) with exponential tail, x^2 exp(-x), and x^2 exp(-x) with exponential tail. For each fit the chi-square per degree of freedom, resolution function parameters and summed neutron widths for the large resonances are listed. The transmission backgrounds and normalizations were fixed at the experimenter's values; that is, the excess normalization and background corrections were set at zero. The spirit of this approach is simple: a mathematical form for the resolution function is assumed, and the transmission data are allowed to choose the width parameters etc. of this form by minimizing chi-square. No prior knowledge of these parameters is assumed; however, the resolution function is constrained by the mathematical form.

The SIOB fits to the ORNL data are straightforward since they crisply converge with *d*, *F*, and *L* all variable. The form x^2 exp (-x) with exponential tail and the form exp($-x^2$) with exponential tail give almost identical results; however, the x^2 exp (-x) form is slightly preferred and is used throughout this work for the ORNL data. The need for an asymmetric resolution function is obvious. This asymmetry tends to increase the resulting neutron widths. For the CBNM and JAERI data sets, the *L* parameter is the major source of confusion in this study.

It is obvious from Table 3 that the JAERI data prefer a Gaussian resolution function with an exponential tail; the chi-square per degree of freedom is very low. The *L* parameter is a real source of confusion and the resulting neutron widths are sensitive to it. For region 3 the fit crisply converges with $L = 142 \pm 13$ mm. For regions 1 and 2 the fits converge with $L = 622 \pm 214$ mm and 211 $\pm$ 32 mm, respectively. These long tails, at least for region 1, act almost as smooth backgrounds which, in this work, will be considered as a separate issue. Consequently, for regions 1 and 2, *L* was simply set at 142 mm. In effect, the assumption is made that the value of *L* from region 3 is correct. The form exp($-x^2$) with exponential tail is used throughout this work for the JAERI data.

The same confusion between long *L*'s and smooth backgrounds exists with the CBNM data. For region 1 the minimum chi-square gives $L = 1032 \pm 591$. As with the JAERI data, the 48-mm value of *L* from region 3 was assumed to be correct. The neutron widths from the CBNM data are not sensitive to small changes (± 10 mm) in small values of *L* (48 mm). The form x^2e^{-x} with exponential tail is clearly preferred over the others and is used throughout this work for the CBNM data.

An examination of the Table 3 results indicates that the summed neutron widths are very sensitive to the assumed form of the resolution function. In all cases the best resolution functions are highly asymmetric and are broader than one would have initially thought. The instrumental resolution for the JAERI data is surprisingly poor. The FWHMs expressed as an equivalent distance are largely independent of energy. In addition, the exponential-tail parameters from the ORNL data are largely independent of energy. More importantly, if the data are analyzed with the same code using the same procedures and are allowed to choose their own resolution function, much of the neutron-width discrepancy is removed if the minimum chi-square resolution functions are chosen. For region 2 the three data sets give an almost identical summed neutron width. The ORNL and CBNM summed widths are in good agreement for region 1 and the ORNL and JAERI summed widths are in good agreement for region 3. However, the JAERI summed width seems about 9% low for region 1 and the CBNM summed width seems about 4% high for region 3. Better agreement with the CBNM results can be obtained if the sample temperatures are increased.

Table 3. SIOB resolution function study with $N = B = 0 \pm 0$

	ORNL (300°K)			CBNM (94.5°K)			JAERI (94.5°K)		
	R-1	R-2	R-3	R-1	R-2	R-3	R-1	R-2	R-3
		$\exp(-x^2)$							
χ^2	1.534	2.280	1.908	3.582	4.188	2.894	0.931	1.528	1.377
d (mm)	54.4 ± 0.4	58.8 ± 0.5	61.7 ± 0.4	43.5 ± 1.0	41.1 ± 0.4	39.7 ± 0.2	140 ± 4	141 ± 2	121 ± 1
F	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0
L (mm)	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0
$\Sigma \Gamma_n$ (eV)	1.413	2.824	2.099	1.417	2.836	2.116	1.266	2.644	1.903
		$\exp(-x^2)$ with tail							
χ^2	1.003	1.066	1.053	2.489	2.444	2.233	0.757	0.908	0.901
d (mm)	27.1 ± 0.6	28.6 ± 0.5	29.3 ± 0.4	34.4 ± 0.9	32.6 ± 0.5	34.0 ± 0.3	124 ± 4	117 ± 2	99 ± 1
F	0.47 ± 0.01	0.42 ± 0.01	0.43 ± 0.01	0.30 ± 0.03	0.23 ± 0.01	0.16 ± 0.01	0.22 ± 0.04	0.22 ± 0.02	0.20 ± 0.01
L (mm)	34 ± 1	36 ± 1	33 ± 1	40 ± 0^a	40 ± 0^a	40 ± 0^a	142 ± 0^b	142 ± 0^b	142 ± 13
$\Sigma\Gamma_n$ (eV)	1.569	3.030	2.184	1.628	3.123	2.291	1.448	2.998	2190
		$x^2\exp(-x)$							
χ^2	1.189	1.513	1.391	2.528	2.131	2.059	1.555	2.271	1.462
d (mm)	55.6 ± 0.5	59.0 ± 0.4	60.5 ± 0.4	44.8 ± 0.8	41.7 ± 0.3	39.8 ± 0.2	137 ± 5	139 ± 3	118 ± 1
F	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0
L (mm)	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0	0 ± 0
$\Sigma\Gamma_n$ (eV)	1499	2.914	2.153	1.525	2.978	2.218	1.307	2.770	1.991
		$x^2\exp(-x)$ with tail							
x^2	1.002	1.031	1.045	2.427	1.949	1.990	1.510	2.051	1.251
d (mm)	33.6 ± 1.1	35.4 ± 0.7	37.2 ± 0.8	38.2 ± 1.1	38.0 ± 0.6	37.6 ± 0.5	113 ± 7	115 ± 5	96 ± 2
F	0.31 ± 0.03	0.26 ± 0.02	0.24 ± 0.01	0.16 ± 0.03	0.09 ± 0.01	0.06 ± 0.01	0.22 ± 0.07	0.18 ± 0.03	0.17 ± 0.01
L (mm)	42 ± 3	46 ± 2	44 ± 2	48 ± 0^b	48 ± 0^b	48 ± 15	135 ± 0^a	135 ± 0^a	135 ± 0^a
$\Sigma\Gamma_n$ (eV)	1.578	3.040	2.190	1.594	3.082	2.278	1.419	3.012	2.204

[a] Arbitrarily chosen.
[b] Fixed at the region-3 value.

5. EFFECTIVE TEMPERATURE CONSIDERATIONS

The fits of Table 3 were performed with effective temperatures of 300°K for the ORNL data and 94.5°K for the CBNM and JAERI data. The resulting neutron widths are sensitive to the input effective temperatures. These sensitivities are illustrated in Table 4 where the percent *decrease* in the summed neutron widths for the nine fits are listed for a 5°K *increase* in effective temperature. As listed, the summed width from the CBNM region 3 data decreases by 0.67% when the effective temperature is raised from 94.5°K to 99.5°K. On the average the neutron widths decrease by 0.88%; the big resonances are less sensitive to temperature than the small resonances. The neutron widths from the ORNL data are considerably less sensitive to temperature than those of CBNM and JAERI.

Table 4. Percent decrease in $\Sigma\Gamma_n$ for a 5°K increase in effective temperature

	R1	R2	R3
ORNL	0.10	0.23	0.14
CBNM	0.97	0.56	0.67
JAERI	0.98	0.71	0.78

For region 3 the effective temperature was externally varied with SIOB, since presently there is no provision to internally vary the effective temperature. One parameter can be varied externally, and the result will be the same if the parameter were internally varied.[11] The region 3 least-squares effective temperatures are listed in Table 5. These fits indicated that the CBNM samples were 21 ± 7°K warmer than those of JAERI.

Table 5. Effective temperatures from fits to region 3

ORNL	301.5 ± 1.5°K
CBNM	108 ± 3°K
JAERI	87 ± 6°K

The prior uncertainty in the effective temperature, assuming the Doppler broadening model is correct, results from the uncertainties in the physical temperature of the sample and in the Debye temperature of the metal. The physical temperature of the ORELA samples is well known (72 ± 5°F, 295.4 ± 2.8°K), whereas those of the CBNM and JAERI samples are probably not so well known but must be greater than 77°K. Moreover, there seems to be confusion in the uranium metal Debye temperature. Jackson and Lynn[12] give a Debye temperature of 165°K whereas the Physics Handbook[13] gives 207°K. These Debye temperatures give effective temperatures of 299°K and 302°K, respectively, for samples at room temperature and 93.2°K and 102.4°K for samples at liquid-nitrogen temperature. The effective temperatures used for the remainder of this study are listed in Table 6. The JAERI value, 94.5°K, is probably the minimum possible effective temperature for uranium metal at liquid nitrogen. The CBNM value is assumed to be 14°K warmer. There is little confusion with the value used for the ORNL data.

Table 6. Effective temperatures used in this study

ORNL	300.0°K
CBNM	108.0°K
JAERI	94.5°K

6. BACKGROUND AND NORMALIZATION CONSIDERATIONS

Tables 7, 8, and 9 list the global parameters (those not for individual resonances) and summed neutron widths for which the excess background and normalization corrections were allowed to vary. The column 1 entries are simply a more complete listing of the Table 3 parameters for the "best" resolution function at the Table 6 effective temperature (only the CBNM results have been changed from Table 3). Column 2 lists the corresponding results in which all the transmissions are renormalized to yield the same effective radius as the ORNL thickest-sample transmission. For the ORNL data this was achieved by fixing the normalization of the 0.175 b^{-1} sample and allowing the radius and normalization of the other samples to vary. For the CBNM and JAERI data this was achieved by fixing the radius at the corresponding ORNL value and allowing the normalization to vary. The normalization of the ORNL 0.175 b^{-1} transmission is known to $\pm 1.5\%$ which, in turn, determines the effective radius to ± 0.04 fm which, in turn, determines the normalizations of the thinner-sample transmissions to a few tenths of a percent.[2] This is largely an academic question since the neutron widths change by less than 1% with this renormalization. Nevertheless, the normalizations of all the thinner-sample transmission data are accurately derived from the ORNL thick-sample transmission.

Column 3 of Tables 7 to 9 lists results with variable excess-background corrections, which are much more interesting and difficult to deal with. These parameters are meant to be a correction to the background which has already been subtracted from the data. For the ORNL data, the excess-background corrections converge to zero within their output uncertainties and, in most cases, the background is determined equal to or better than was done experimentally. More importantly, there is no difference in the neutron widths and their uncertainties if the excess background corrections are fixed at zero or varied! This is an important result since the fits give the same backgrounds as were measured and the uncertainties in the measured backgrounds have almost no effect on the resulting neutron widths.

For the CBNM and JAERI data the results are not so nice. At all energies additional background is subtracted from the data at the minima chi-square which, in turn, increases the resulting neutron widths. At all energies, this increases the neutron width differences with the ORNL results. In region 3 the neutron widths are increased by 1 to 2% with additional background subtractions of 1 to 2%, and in region 1 the neutron widths are increased by 40% with additional background subtractions from 10 to 20%.

The last column of Tables 7 to 9 gives a variety of results, depending on the data set. For the ORNL data, the last column lists parameters for the case when even the normalization of the thickest sample is allowed to vary. For regions 2 and 3, this variable has little effect on the resulting neutron widths or their uncertainties. For region 1, this variable has some effect. However, the normalization correction is larger than the 1.5% published uncertainty[2] in this parameter.

Table 7. SIOB normalization and background study for region 1

ORNL (300°K)				
χ^2	1.0019	0.9985	0.9979	0.9967
d (mm)	33.6 ± 1.1	33.4 ± 1.1	32.9 ± 2.0	32.0 ± 2.1
F	0.312 ± 0.024	0.313 ± 0.025	0.323 ± 0.026	0.339 ± 0.031
L (mm)	41.7 ± 3.1	41.3 ± 3.1	39.7 ± 3.5	36.2 ± 3.6
N(0.004)	0 ± 0	0.0008 ± 0.0016	0.0017 ± 0.0017	0.0005 ± 0.0018
N(0.012)	0 ± 0	−0.0001 ± 0.0017	0.0006 ± 0.0018	−0.0032 ± 0.0026
N(0.053)	0 ± 0	−0.0062 ± 0.0021	−0.0061 ± 0.0023	−0.0205 ± 0.0073
N(0.175)	0 ± 0	0 ± 0	0 ± 0	−0.0445 ± 0.0210
B(0.004)	0 ± 0	0 ± 0	−0.0240 ± 0.0177	−0.0061 ± 0.0189
B(0.012)	0 ± 0	0 ± 0	−0.0045 ± 0.0068	0.0072 ± 0.0083
B(0.053)	0 ± 0	0 ± 0	0.0013 ± 0.0024	0.0054 ± 0.0030
B(0.175)	0 ± 0	0 ± 0	0.0007 ± 0.0005	0.0011 ± 0.0006
R (fm)	10.001 ± 0.007	9.993 ± 0.007	9.996 ± 0.008	9.89 ± 0.05
S	−0.04 ± 0.06	−0.07 ± 0.06	−0.08 ± 0.06	−0.09 ± 0.06
$\Sigma\Gamma_n$ (eV)	1.578	1.570	1.572	1.592
CBNM (108°K)				
χ^2	2.501	2.471	2.099	2.130
d (mm)	38.4 ± 1.2	38.4 ± 1.2	36.6 ± 1.3	38.9 ± 1.0
F	0.16 ± 0.03	0.16 ± 0.04	0.09 ± 0.04	0.12 ± 0.09
L(mm)	48 ± 0	48 ± 0	48 ± 0	380 ± 361
N(0.035)	0 ± 0	0.0091 ± 0.0029	−0.0067 ± 0.0044	0.0027 ± 0.0098
N(0.014)	0 ± 0	0.0007 ± 0.0021	−0.0046 ± 0.0029	−0.0003 ± 0.0050
B(0.035)	0 ± 0	0 ± 0	0.118 ± 0.017	0.078 ± 0.051
B(0.014)	0 ± 0	0 ± 0	0.176 ± 0.028	0.117 ± 0.074
R (fm)	9.90 ± 0.03	9.99 ± 0	9.99 ± 0	9.99 ± 0
S	0.02 ± 0.23	0.04 ± 0.24	0.90 ± 0.33	0.49 ± 0.35
$\Sigma\Gamma_n$ (eV)	1.558	1.550	2.016	2.006
JAERI (94.5°)				
χ^2	0.757	0.753	0.739	0.676
d (mm)	124 ± 4	123 ± 4	112 ± 6	118 ± 5
F	0.22 ± 0.04	0.22 ± 0.04	0.22 ± 0.05	0.27 ± 0.09
L (mm)	142 ± 0	142 ± 0	142 ± 0	497 ± 251
N(0.014)	0 ± 0	0.004 ± 0.002	−0.002 ± 0.004	0.010 ± 0.007
B(0.014)	0 ± 0	0 ± 0	0.192 ± 0.058	0.095 ± 0.089
R (fm)	9.89 ± 0.06	9.99 ± 0	9.99 ± 0	9.99 ± 0
S	−0.6 ± 0.4	−0.6 ± 0.4	0.4 ± 0.6	−0.5 ± 0.7
$\Sigma\Gamma_n$ (eV)	1.448	1.459	2.071	2.040

Table 8. SIOB normalization and background study for region 2

ORNL (300°K)				
χ^2	1.0312	1.0231	1.0190	1.0194
d (mm)	35.4 ± 0.7	35.4 ± 0.7	36.4 ± 0.7	36.4 ± 0.7
F	0.263 ± 0.012	0.263 ± 0.012	0.244 ± 0.012	0.244 ± 0.011
L (mm)	46.5 ± 1.8	46.2 ± 1.8	50.0 ± 2.4	50.2 ± 2.4
N(0.004)	0 ± 0	0.0001 ± 0.0011	0.0006 ± 0.0012	0.0006 ± 0.0012
N(0.012)	0 ± 0	0.0000 ± 0.0012	−0.0002 ± 0.0012	0.0000 ± 0.0014
N(0.053)	0 ± 0	−0.0067 ± 0.0015	−0.0059 ± 0.0015	−0.0052 ± 0.0027
N(0.175)	0 ± 0	0 ± 0	0 ± 0	0.0021 ± 0.0071
B(0.004)	0 ± 0	0 ± 0	0.0075 ± 0.0057	0.0069 ± 0.0058
B(0.012)	0 ± 0	0 ± 0	0.0019 ± 0.0024	0.0017 ± 0.0025
B(0.053)	0 ± 0	0 ± 0	−0.0026 ± 0.0010	−0.0027 ± 0.0011
B(0.175)	0 ± 0	0 ± 0	−0.0001 ± 0.0004	−0.0001 ± 0.0004
R (fm)	9.790 ± 0.005	9.780 ± 0.006	9.779 ± 0.006	9.78 ± 0.02
S	0.26 ± 0.03	0.25 ± 0.03	0.26 ± 0.03	0.26 ± 0.03
$\Sigma\Gamma_n$ (eV)	3.040	3.032	3.036	3.034
CBNM (108°K)				
χ^2	1.969	1.937	1.844	1.812
d (mm)	38.0 ± 0.6	37.8 ± 0.6	37.7 ± 0.6	38.4 ± 0.5
F	0.089 ± 0.012	0.099 ± 0.012	0.065 ± 0.015	0.071 ± 0.015
L (mm)	48 ± 0	48 ± 0	48 ± 0	133 ± 53
N(0.035)	0 ± 0	0.0120 ± 0.0017	0.0099 ± 0.0018	0.0124 ± 0.0021
N(0.014)	0 ± 0	0.0038 ± 0.0012	0.0032 ± 0.0013	0.0049 ± 0.0015
B(0.035)	0 ± 0	0 ± 0	0.0247 ± 0.0055	0.0105 ± 0.0087
B(0.014)	0 ± 0	0 ± 0	0.0304 ± 0.0089	0.0093 ± 0.0135
R (fm)	9.64 ± 0.02	9.78 ± 0	9.78 ± 0	9.78 ± 0
S	0.17 ± 0.10	0.27 ± 0.10	0.32 ± 0.11	0.31 ± 0.10
$\Sigma\Gamma_n$ (eV)	3.031	3.046	3.148	3.136
JAERI (94.5°K)				
χ^2	0.908	0.884	0.882	0.854
d (mm)	117.4 ± 1.8	115.6 ± 1.8	111.7 ± 2.2	114.5 ± 2.3
F	0.220 ± 0.015	0.238 ± 0.015	0.224 ± 0.017	0.219 ± 0.017
L (mm)	142 ± 0	142 ± 0	142 ± 0	207 ± 32
N(0.014)	0 ± 0	0.0109 ± 0.0014	0.0105 ± 0.0015	0.0125 ± 0.0017
B(0.014)	0 ± 0	0 ± 0	0.0430 ± 0.0160	0.0184 ± 0.0193
R (fm)	9.49 ± 0.04	9.78 ± 0	9.78 ± 0	9.78 ± 0
S	−0.39 ± 0.19	−0.19 ± 0.19	−0.69 ± 0.20	−0.69 ± 0.20
$\Sigma\Gamma_n$ (eV)	2.998	3.024	3.221	3.187

Table 9. SIOB normalization and background study for region 3

ORNL (300°K)				
χ^2	1.0474	1.0386	1.0389	1.0416
d (mm)	36.6 ± 0.8	36.8 ± 0.8	34.9 ± 0.9	35.0 ± 1.1
F	0.246 ± 0.014	0.248 ± 0.015	0.279 ± 0.019	0.275 ± 0.019
L (mm)	43.7 ± 2.0	43.2 ± 1.9	37.8 ± 2.2	38.2 ± 2.3
N(0.004)	0 ± 0	0.0015 ± 0.0008	0.0012 ± 0.0009	0.0013 ± 0.0009
N(0.012)	0 ± 0	0.0011 ± 0.0008	0.0006 ± 0.0009	0.0009 ± 0.0010
N(0.053)	0 ± 0	−0.0052 ± 0.0010	−0.0057 ± 0.0010	−0.0043 ± 0.0025
N(0.175)	0 ± 0	0 ± 0	0 ± 0	0.0046 ± 0.0075
B(0.004)	0 ± 0	0 ± 0	0.0071 ± 0.0040	0.0065 ± 0.0041
B(0.012)	0 ± 0	0 ± 0	0.0052 ± 0.0018	0.0048 ± 0.0019
B(0.053)	0 ± 0	0 ± 0	0.0025 ± 0.0009	0.0023 ± 0.0009
B(0.175)	0 ± 0	0 ± 0	0.0002 ± 0.0003	0.0002 ± 0.0003
R (fm)	9.507 ± 0.004	9.501 ± 0.004	9.500 ± 0.004	9.51 ± 0.02
S	0.166 ± 0.016	0.166 ± 0.016	0.165 ± 0.016	0.167 ± 0.016
$\Sigma\Gamma_n$ (eV)	2.186	2.182	2.182	2.180
CBNM (108°K)				
χ^2	1.988	1.939	1.862	
d (mm)	37.4 ± 0.5	37.1 ± 0.4	37.5 ± 0.4	
F	0.062 ± 0.014	0.074 ± 0.008	0.031 ± 0.011	
L (mm)	48 ± 15	48 ± 0	48 ± 0	
N(0.035)	0 ± 0	0.0142 ± 0.0010	0.0131 ± 0.0011	
N(0.014)	0 ± 0	0.0059 ± 0.0008	0.0054 ± 0.0008	
B(0.035)	0 ± 0	0 ± 0	0.0224 ± 0.0032	
B(0.014)	0 ± 0	0 ± 0	0.0245 ± 0.0052	
R (fm)	9.32 ± 0.02	9.50 ± 0	9.50 ± 0	
S	0.23 ± 0.05	0.20 ± 0.06	0.27 ± 0.06	
$\Sigma\Gamma_n$ (eV)	2.236	2.253	2.294	
JAERI (94.5°K)				
χ^2	0.900	0.898	0.895	
d (mm)	99.3 ± 1.1	98.8 ± 1.2	96.0 ± 1.5	
F	0.199 ± 0.010	0.206 ± 0.011	0.210 ± 0.013	
L (mm)	142 ± 13	141 ± 13	115 ± 13	
N(0.014)	0 ± 0	0.0043 ± 0.0008	0.0035 ± 0.0009	
B(0.014)	0 ± 0	0 ± 0	0.0211 ± 0.0078	
R (fm)	9.37 ± 0.03	9.50 ± 0	9.50 ± 0	
S	0.42 ± 0.10	0.45 ± 0.10	0.43 ± 0.10	
$\Sigma\Gamma_n$ (eV)	2.190	2.194	2225	

For the CBNM and JAERI data, the last column of Tables 7 and 8 lists results when both *B* and *L* are varied. The chi-square minima occur for large values of *L* and corresponding excess-background corrections which yield neutron widths and uncertainties which are very similar to those of column 3, constrained values of *L* with excess background corrections. The long exponential tails act as smooth backgrounds so ultimately the questions of excess background corrections and resolution functions are coupled. With no constraints on the resolution function, excess background and normalization corrections, the last column of Tables 7 to 9 gives the best least-squares fits to the three data sets.

Tables 10, 11, and 12 compare the resulting neutron widths from this work with the corresponding published values. For the ORNL data, only the column 2 neutron widths from Tables 7 to 9 are listed since the variable backgrounds make no difference. For the CBNM and JAERI data, the column 2 neutron widths are listed under the "$B=0$" heading and the column 3 or 4 neutron widths are listed under the "$B\neq0$" heading. The large uncertainties in the 1979 published ORNL neutron widths[2] were required to cover various systematic discrepancies observed from the fits at that time. With the improved analysis and understanding developed over the following five years and discussed in this report, these systematic discrepancies no longer exist.

7. ORNL AND CBNM NEUTRON WIDTHS FROM SINGLE-SAMPLE FITS

The four ORNL transmissions were simultaneously least-squares fitted, as well as the two CBNM transmissions. The question naturally arises of how the neutron widths compare from the individual samples if they are fitted separately. The results of such fits are listed in Table 13. For these calculations the global parameters (*d, F, L, N,* $B=0$, *R*, and *S*) were all fixed at the column 2 values of Tables 7 to 9; that is, the zero excess-background case. Only the resonance energies and neutron widths were varied. The results listed in Table 13 are very gratifying, particularly for the ORNL data. There are almost no systematic differences between the neutron widths from the different samples. Moreover, on a resonance-by-resonance basis the agreement is good. As a point of reference, Table 14 from ref. 14 shows such a comparison made in 1976 using an area analysis code[15] with the ORNL 40-m data.[14] The good agreement in Table 13 gives considerable confidence that the whole procedure and global parameters from the present work are valid.

With the CBNM data there seems to be some tendency for thinner samples to give larger neutron widths than the thicker sample. Moreover, the chi-square for the thick sample is much, much smaller than that for the thin sample, even with the uncertainties about the same for both samples. In addition, the thicker sample neutron widths agree better with those of ORNL and JAERI than do those of the thinner sample. The origin of this problem is not clearly understood. As a final check, the two CBNM samples were fit separately, with the global parameters allowed to vary. The difference between these results and those of Table 13 are not large enough to warrant discussion for regions 2 and 3. For region 1 the difference is confusing and substantial. No attempt was made to determine if the two samples were at different temperatures. In any event, there are no serious problems with the results listed in Table 13.

8. DISCUSSION OF NEUTRON WIDTHS

Table 15 compares the neutron widths given in Tables 10 to 12 as percentage deviations from those of ENDF/B-V.[8] Differences are listed in terms of the average of the deviations on a resonance-by-resonance basis. These deviations are plotted in Fig. 11 and connected by straight lines. The three smallest resonances in both Tables 11 and 12 have not been included in the averages since the deviations can be very large and still be statistically consistent. The ORNL neutron widths from the present

Table 10. Neutron widths (meV) for region 1

E (eV)	ORNL Published	ORNL 1983	CBNM Published	CBNM SIOB $B=0$	CBNM SIOB $B\neq0$	JAERI Published	JAERI SIOB $B=0$	JAERI SIOB $B\neq0$
3858	609 ± 33	624 ± 4	623 ± 40	617 ± 16	815 ± 38	482 ± 42	598 ± 22	848 ± 95
3873	178 ± 13	188 ± 3	165 ± 12	191 ± 10	240 ± 14	159 ± 19	183 ± 13	243 ± 29
3902	303 ± 18	314 ± 3	285 ± 25	317 ± 12	421 ± 23	248 ± 25	283 ± 15	409 ± 50
3915	114 ± 8	123 ± 2	85 ± 10	118 ± 7	143 ± 10	100 ± 12	115 ± 9	145 ± 17
3940	174 ± 12	179 ± 3	195 ± 20	173 ± 9	225 ± 15	142 ± 16	157 ± 12	224 ± 29
3955	134 ± 9	142 ± 2	105 ± 11	135 ± 9	162 ± 11	110 ± 15	123 ± 11	170 ± 20
Sum	1512	1570	1458	1550	2006	1241	1459	2040

Table 11. Neutron widths (meV) for region 2

E (eV)	ORNL Published	ORNL 1983	CBNM Published	CBNM SIOB $B=0$	CBNM SIOB $B\neq0$	JAERI Published	JAERI SIOB $B=0$	JAERI SIOB $B\neq0$
2489	106 ± 6	111.0 ± 1.2	109 ± 6	120 ± 4	124 ± 4	104 ± 8	118 ± 5	125 ± 6
2521	20.2 ± 1.5	21.2 ± 0.4	19 ± 4	25 ± 2	25 ± 2		24 ± 2	24 ± 2
2548	748 ± 38	755 ± 3	703 ± 30	756 ± 6	780 ± 9		727 ± 10	766 ± 21
2559	295 ± 16	310.7 ± 1.8	270 ± 15	318 ± 5	321 ± 6		321 ± 8	334 ± 11
2581	461 ± 24	474.2 ± 2.0	391 ± 16	467 ± 6	477 ± 7		491 ± 10	508 ± 15
2598	768 ± 40	784 ± 4	727 ± 42	785 ± 7	818 ± 11		771 ± 12	822 ± 24
2620	49 ± 4	49.1 ± 1.0	44 ± 5	49 ± 3	50 ± 3		58 ± 3	61 ± 4
2672	297 ± 16	303.7 ± 2.0	269 ± 16	296 ± 5	305 ± 6	256 ± 21	293 ± 9	312 ± 11
2696	34 ± 3	35.2 ± 0.7	28 ± 3	33 ± 2	34 ± 2	28 ± 4	38 ± 3	39 ± 3
2717	183 ± 10	187.6 ± 1.6	157 ± 11	196 ± 5	202 ± 5	170 ± 17	184 ± 7	195 ± 8
Sum	2961	3032	2717	3046	3136		3024	3187

Table 12. Neutron widths (meV) for region 3

E (eV)	ORNL Published	ORNL 1983	CBNM Published	CBNM SIOB $B=0$	CBNM SIOB $B\neq0$	JAERI Published	JAERI SIOB $B=0$	JAERI SIOB $B\neq0$
1474	120 ± 5	125.6 ± 0.8	125 ± 5	131.4 ± 2.1	133.1 ± 2.1	123 ± 8	131 ± 3	133 ± 4
1523	245 ± 11	253.7 ± 1.3	246 ± 10	257.3 ± 2.6	262.7 ± 2.8	237 ± 14	258 ± 4	263 ± 5
1598	379 ± 16	387.0 ± 1.4	410 ± 30	392.3 ± 3.1	401.3 ± 3.5	378 ± 30	380 ± 5	386 ± 6
1623	98 ± 5	102.6 ± 0.8	114 ± 5	111.8 ± 2.1	113.0 ± 2.2	104 ± 13	107 ± 3	108 ± 3
1638	49.5 ± 2.6	52.7 ± 0.6	55 ± 3	56.6 ± 1.5	56.6 ± 1.5	46 ± 5	56 ± 2	57 ± 2
1662	226 ± 10	230.5 ± 1.2	220 ± 10	242.3 ± 2.9	246.4 ± 3.0	211 ± 19	214 ± 4	217 ± 5
1689	107 ± 5	109.0 ± 0.9	108 ± 4	114.3 ± 2.2	115.3 ± 2.3	103 ± 9	106 ± 3	107 ± 3
1710	91 ± 4	91.2 ± 0.8	95 ± 10	93.9 ± 2.0	94.5 ± 2.0	86 ± 8	88 ± 3	89 ± 3
1723	17.8 ± 1.1	18.2 ± 0.3	19.8 ± 1.6	19.7 ± 0.8	19.6 ± 0.9	19 ± 3	18.6 ± 1.0	18.5 ± 1.0
1756	140 ± 6	141.1 ± 1.0	140 ± 6	147.3 ± 2.6	148.1 ± 2.6	139 ± 10	152 ± 4	154 ± 4
1783	664 ± 27	651 ± 3	652 ± 30	666 ± 4	683 ± 5	697 ± 72	664 ± 7	675 ± 9
1808	19.2 ± 1.3	19.5 ± 0.4	20.5 ± 2.0	20.1 ± 0.9	20.1 ± 0.9	21 ± 4	18.2 ± 1.1	18.2 ± 1.1
Sum	2157	2182	2205	2253	2294	2164	2194	2225

Table 13. Comparison of ORNL and CBNM neutron widths from the simultaneous fits to all samples and from individual sample fits

	ORNL					CBNM		
	All samples	0.175 b^{-1}	0.052 b^{-1}	0.012 b^{-1}	0.0038 b^{-1}	All samples	0.035 b^{-1}	0.010 b^{-1}
Region 1								
3858	624 ± 4	621 ± 4	619 ± 7	630 ± 11	669 ± 19[a]	617 ± 16	602 ± 9	660 ± 21
3873	188 ± 3	188 ± 3	190 ± 4	185 ± 6	183 ± 13	191 ± 10	200 ± 8	196 ± 14
3902	314 ± 3	315 ± 3	311 ± 5	317 ± 7	294 ± 15	317 ± 12	315 ± 9	332 ± 18
3915	123 ± 2	122 ± 3	123 ± 3	126 ± 5	134 ± 13	118 ± 7	124 ± 7	120 ± 12
3940	179 ± 3	176 ± 3	180 ± 4	185 ± 6	169 ± 14	173 ± 9	173 ± 8	183 ± 15
3955	142 ± 2	136 ± 3	146 ± 3	148 ± 5	147 ± 13	135 ± 9	142 ± 8	137 ± 13
Sum	1570	1558	1569	1591	1596	1550	1556	1628
Region 2								
2489	111.0 ± 1.2	110.3 ± 1.5	112.0 ± 2.2	110.9 ± 2.6	110 ± 7	120 ± 4	113 ± 4	126 ± 5
2521	21.2 ± 0.4	20.6 ± 0.5	22.1 ± 0.6	21.1 ± 1.7	28 ± 6	25 ± 2	25 ± 2	27 ± 3
2548	755 ± 3	749 ± 3	761 ± 4	761 ± 8	760 ± 13	756 ± 6	742 ± 6	773 ± 9
2559	310.7 ± 1.8	314.2 ± 2.0	313 ± 4	303 ± 5	271 ± 9[a]	318 ± 5	311 ± 5	328 ± 8
2581	474.2 ± 2.0	471.4 ± 2.3	479 ± 4	476 ± 7	478 ± 11	467 ± 6	468 ± 5	467 ± 8
2598	784 ± 4	784 ± 4	789 ± 5	766 ± 8	763 ± 14	785 ± 7	780 ± 6	790 ± 8
2620	49.1 ± 1.0	51.5 ± 3.0	50.0 ± 1.2	45.8 ± 2.1	43 ± 6	49 ± 3	50 ± 3	49 ± 4
2672	303.7 ± 2.0	306.2 ± 2.3	304.5 ± 3.6	298 ± 5	275 ± 9[a]	296 ± 5	302 ± 5	289 ± 8
2696	35.2 ± 0.7	36.0 ± 1.5	34.5 ± 0.9	38.6 ± 2.1	37 ± 7	33 ± 2	38 ± 2	27 ± 3
2717	187.6 ± 1.6	185.8 ± 2.0	194.4 ± 3.1	183.8 ± 3.6	191 ± 8	196 ± 5	197 ± 5	197 ± 7
Sum	3032	3029	3060	3004	2956	3046	3026	3073
Region 3								
1474	125.6 ± 0.8	126.2 ± 1.0	124.2 ± 1.8	127.2 ± 2.0	127 ± 3	131.4 ± 2.1	127.7 ± 1.8	135 ± 3
1523	253.7 ± 1.3	256.3 ± 1.5	251.9 ± 2.1	250 ± 3	249 ± 4	257.3 ± 2.6	252.9 ± 2.2	263 ± 4
1598	387.0 ± 1.4	388.8 ± 1.9	384.4 ± 2.5	389 ± 4	379 ± 6	392.3 ± 3.1	383.4 ± 2.5	403 ± 5
1623	102.6 ± 0.8	104.2 ± 1.1	100.0 ± 1.6	102.5 ± 1.7	98 ± 3	111.8 ± 2.1	107.9 ± 2.0	116 ± 3
1638	52.7 ± 0.6	53.6 ± 0.9	52.7 ± 1.0	51.0 ± 1.2	55 ± 3	56.6 ± 1.5	57.3 ± 1.5	56.1 ± 2.0
1662	230.5 ± 1.2	230.4 ± 1.4	230.1 ± 2.2	233 ± 4	235 ± 5	242.3 ± 2.9	241.1 ± 2.4	245 ± 5
1689	109.0 ± 0.9	109.0 ± 1.1	111.2 ± 1.8	106.9 ± 2.0	104 ± 4	114.3 ± 2.2	113.9 ± 2.1	115 ± 3
1710	91.2 ± 0.8	89.5 ± 1.1	96.1 ± 1.6[a]	89.7 ± 1.6	91 ± 4	93.9 ± 2.0	96.5 ± 2.0	91 ± 3
1723	18.2 ± 0.3	18.2 ± 0.7	18.3 ± 0.4	17.9 ± 1.0	18 ± 3	19.7 ± 0.8	19.0 ± 0.7	20.9 ± 1.6
1756	141.1 ± 1.0	140.0 ± 1.1	146.7 ± 2.0[a]	140.4 ± 2.3	137 ± 4	147.3 ± 2.6	150.1 ± 2.4	143 ± 4
1783	651 ± 3	651 ± 3	649 ± 3	651 ± 6	674 ± 9[a]	666 ± 4	658 ± 4	674 ± 6
1808	19.5 ± 0.4	18.3 ± 1.1	19.4 ± 0.5	20.0 ± 1.1	18 ± 3	20.1 ± 0.9	20.0 ± 0.8	20.5 ± 1.6
Sum	2182	2186	2184	2179	2185	2253	2227	2282

[a]More than two standard deviations from the all-sample value.

Table 14. 1976 area analysis of ORNL 40-m transmission data[a]

					ORNL				
Energy	ENDF/B-IV	Columbia[6]	Geel[7]	JAERI[4]	Weighted[b]	0.425	0.100	0.30	0.01
2547.2	550	550 ± 50	734 ± 50	-	643 ± 31	632 ± 20	623 ± 45	639 ± 49	717 ± 80
2558.5	230	230 ± 30	234 ± 15	-	230 ± 15	262 ± 19	232 ± 19	227 ± 28	223 ± 67
2579.9	330	340 ± 30	410 ± 30	-	380 ± 23	364 ± 17	383 ± 33	399 ± 36	314 ± 62
2596.5	670	740 ± 45	786 ± 60	-	689 ± 33	860 ± 22	675 ± 45	701 ± 53	694 ± 95
2671.3	240	270 ± 20	275 ± 20	256 ± 21	243 ± 19	297 ± 19	245 ± 25	251 ± 32	192 ± 65
2716.5	145	145 ± 29	170 ± 15	179 ± 17	172 ± 15	165 ± 15	183 ± 18	154 ± 26	152 ± 58
$\Sigma\Gamma_n$	2165	2275 ± 85	2609 ± 89	-	2357 ± 58	2580 ± 46	2341 ± 80	2371 ± 95	2291 ± 177

[a]Neutron widths in meV from area analyses of the large ^{238}U resonances between 2500 and 2800 eV.

[b]These results labeled ORNL are the weighted means of the widths in columns 8, 9, and 10 from the 100-, 30-, and 10-mil samples respectively.

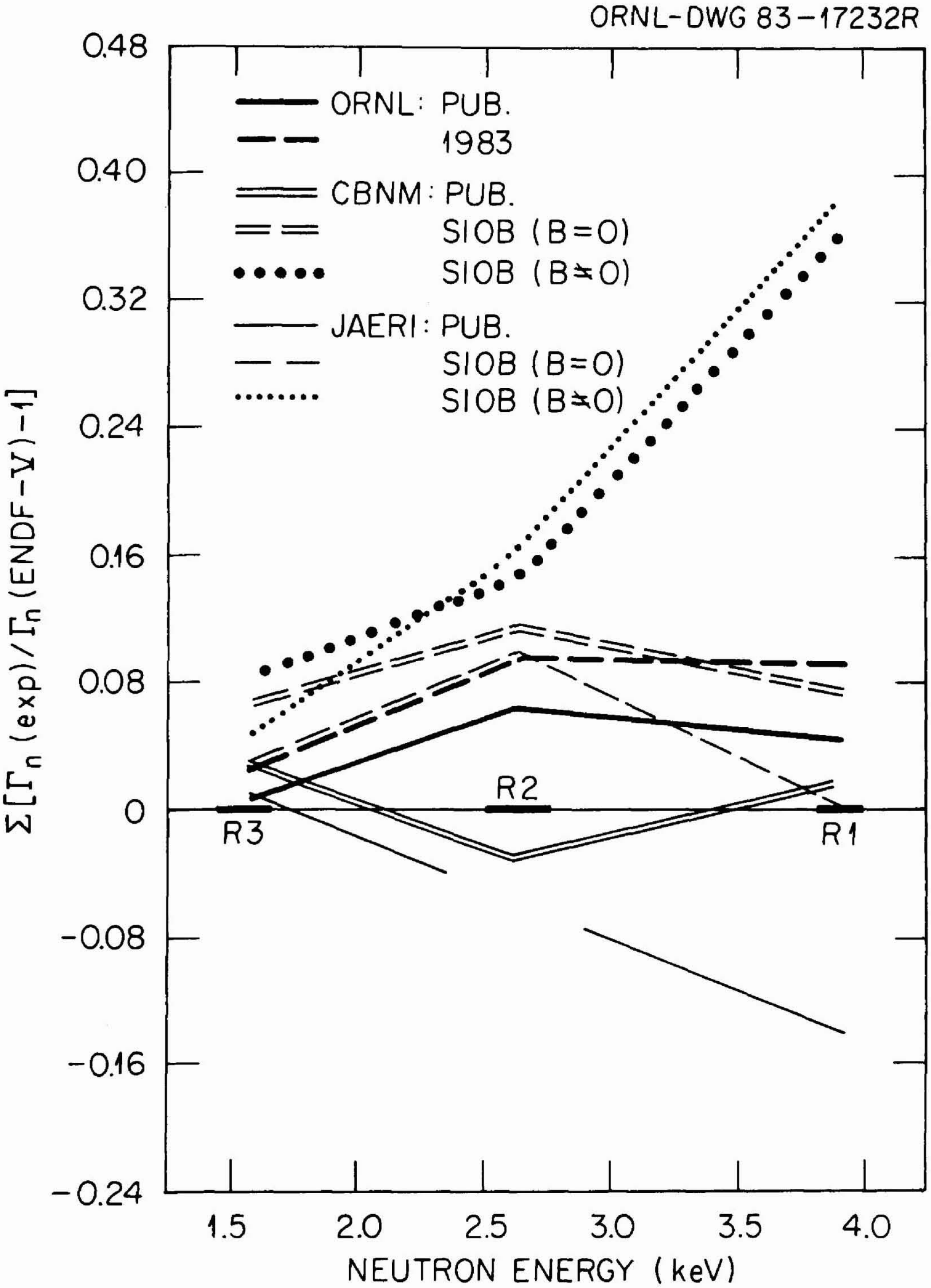

Fig. 11. Average deviations from the ENDF/B-V evaluation for the published and SIOB-fitted neutron widths from the three data sets. The deviations for the three energy regions are connected with straight lines. The dashed lines are results with no excess-background corrections and, the dotted lines are results with variable excess-background corrections.

Table 15. Neutron width percentage deviations from the ENDF-V evaluation. The entries are the average deviation on a resonance by resonance bases.

		R1	R2	R3
ORNL:	Published	4.2	6.2	0.5
	1983	9.2	9.4	2.4
CBNM:	Published	−4.1	−2.3	3.7
	SIOB (B=0)	7.2	11.1	6.5
	SIOB (B≠0)	36.1	14.5	8.1
JAERI:	Published	−12.8		−0.3
	SIOB (B=0)	0.4	9.8	3.0
	SIOB (B≠0)	37.9	15.7	4.4

SIOB fits have been increased by 5, 3, and 2% for regions 1, 2, and 3, respectively, over those previously published.[2] These increases result from allowing the resolution function parameters to be fitting variables and the correction of a coding error connected to the folding of the exponential tail function. These increases are within the systematic uncertainties of the published widths.[2]

Two sets of neutron widths are shown from the CBNM and JAERI data. The dashed lines are results for excess-background corrections fixed at zero and the dotted lines are results with variable excess-background corrections. There is a very big difference in the two sets of widths. In all cases the variable excess-background corrections converge to positive values, which subtracts more background from the experimental data, increases the resulting neutron widths, and increases the systematic differences with the ORNL results. About 4% backgrounds were initially subtracted from the CBNM raw data.[3] The chi-square minima occur when 2.0 to 3.0% more background is subtracted from regions 2 and 3, and 12 to 18% more background is subtracted from region 1. It is impossible to believe that the CBNM background estimate is off by a factor of 4! Because of this inconsistency and the belief that the excess-background corrections are more a measure of slight imperfections in assumed resolution function forms than a true measure of background errors, it is put forth here that the most reliable neutron widths from this work are those when the excess background corrections have been fixed at zero. If the resolution functions are very well determined, or if the transmission data contain very black resonances, or if the data are insensitive to the resolution function, then variable excess-background corrections may have physical meaning. It is important to note that a Bayesian approach may not completely solve this problem. It would only constrain the excess-background corrections which could still be influenced by imperfect resolution functions. Fortunately, variable excess background corrections make no difference to the ORNL neutron widths. This very pleasing result stems from three factors:

1. The transmissions contain many very black resonances, which tend to determine the background independent of the resolution function.
2. The multitude of samples tends to sort out better the excess-background corrections and the resolution function parameters.

3. The resulting neutron widths are less sensitive to the resolution function. At 4 keV the ORNL transmission dips result from folding a 2-eV-wide Doppler width with a 2-eV-wide resolution width, whereas the CBNM and JAERI transmission dips result from folding a 1-eV-wide Doppler width with a 5-eV-wide resolution width.

This latter point is important. If the two thinnest ORNL samples are fitted together in region 1, a summed width of 1.535 eV results with excess background corrections of -4 ± 3% and -7 ± 5%. That is, a 2.4% reduction in the summed width is obtained while adding more background to the data than was originally subtracted. Clearly, variable excess-background corrections must be treated with a great deal of care and in some cases a great deal of skepticism.

The most consistent neutron widths from this work are those with the excess-background corrections fixed at zero. In this case, the systematic differences between the three sets of neutron widths have been substantially reduced with the present SIOB fits. As shown in Fig. 11, the systematic differences between the ORNL and JAERI widths for regions 2 and 3 are negligible. The CBNM widths are 2% smaller and 2% larger than those of ORNL in regions 1 and 2, respectively. In region 1 the JAERI widths are 8% smaller than those of ORNL and CBNM; almost surely, this is some sort of background subtraction confusion. If only 4% more backgrond were subtracted from the JAERI data in region 1, the resulting widths would be consistent. Somewhat surprisingly, the CBNM widths are 4% larger than those of ORNL and JAERI in region 3. The origin of this discrepancy is not clearly understood, but may be a resolution function problem. The large chi-square for the thin sample in this region may indicate that the resolution function form used in this study is not optimum. Perhaps the two samples should not have been fit simultaneously. In any event it seems obvious that some sort of weighted average of SIOB-extracted neutron widths from the ORNL and CBNM data up to 4 keV and JAERI data up to 3 keV would have a demonstrated systematic uncertainty of less than or equal to 3%.

9. PROBLEMS WITH UNCERTAINTIES

There are many problems associated with the neutron-width uncertainties listed in this work. The average SIOB-output neutron-width uncertainties listed in Tables 10 to 12 from the ORNL data, excluding the six smallest resonances, are 1.33, 0.62, and 0.62% for regions 1, 2, and 3, respectively. If the normalization of the 0.175 b^{-1} sample and all the excess background corrections are allowed to vary, these average uncertainties increase to 1.45, 0.64, and 0.65%, respectively. These latter uncertainties assume no prior knowledge in *d, F, L, N,* and *B*. The excess-background and normalization corrections all converge to reasonable values with uncertainties more or less smaller than or equivalent to those determined experimentally except for the normalization of the thickest sample and the background of the thinnest sample in region 1. Inspection of Tables 4 to 6 indicate that the effective-temperature uncertainty for the ORNL data is not a factor in the present problem. In addition, the prior uncertainties in the sample thickness and capture widths are not a factor. The sample thicknesses are known to ±0.10%. If all four sample thicknesses are increased by 0.10%, the average neutron widths in region 3 decrease by 0.14%. Similarily, if all the region 3 capture widths are increased by 10%, the average neutron width increases by 0.04%. Clearly these uncertainties can be neglected.

A problem which perhaps should not be neglected is the fact that the ORNL transmission uncertainties are partially correlated over sample thickness, since all the sample-in spectra are normalized to the same sample-out spectrum. SIOB presently treats these transmission spectra as being statistically independent. Because of this the uncertainties in the all-sample fits prior to multiplication by χ^2 are substantially underestimated. On the average, the neutron-width uncertainties need to be multiplied by approximately 1.3. Logically consistent uncertainty estimates would require a fix to this problem. Nevertheless, the ORNL data determine the neutron widths of the major resonances below 4 keV with an accuracy in the order of 2% or less. A Bayesian fit to each energy region with prior non-fitting uncertainties on the global parameter would not significantly alter the neutron-width uncertainties.

The major fitting problem with the CBNM and JAERI data is the confusion between resolution function and background and the occurrence of chi-square minima with appreciable excess-background corrections. Moreover, the results listed in Tables 4 to 6 indicate that the effective temperature uncertainties should perhaps be accounted for correctly. This would seem to require a full Bayesian analysis on a successive region-by-region basis with reliable prior uncertainties on the temperature and excess-background corrections. The resolution-function tail parameter would still have to be determined at low energies and assumed constant into the higher energies. Moreover, there is some indication that the resolution-function form for the CBNM data is not optimum or that the two samples should not be simultaneously fitted. A better resolution function could be obtained only with Monte Carlo calculations or a trial-and-error approach seeking a lower chi square. The average neutron-width uncertainties from the CBNM data for the zero excess-background correction fits are 4.9, 1.7, and 1.4% for regions 1, 2, and 3, respectively. For the JAERI data the corresponding uncertainties are 6.8, 2.7, and 2.2%. A proper Bayesian analysis could only increase these uncertainties. In any inverse variance weighted average, the neutron widths from the ORNL data would roughly outweigh on the average those of CBNM and JAERI by a factor of ten.

10. RECOMMENDATIONS

Any discussion for recommendations for future measurements and analyses depends on the neutron-width accuracy requirements, the time span to complete the task, the energy range under discussion, and the question of verification. It is one thing to desire a single measurement to give neutron widths within a given uncertainty. It is a more difficult requirement to ask several measurements to give demonstrated agreement within that uncertainty. Over the next year or two it is probably safe to assume that the data base will not expand appreciably. Hence, in the short term we are left with analyzing the present data with existing or improved codes. Above 4 keV the resulting neutron widths would have to depend almost entirely on the ORNL data. In the long term, new measurements could be completed.

10.1 CODE RECOMMENDATIONS

The author is familiar only with the analysis codes at ORNL, of which only two are presently relevant: SIOB[2,5] and SAMMY.[16] SIOB has the advantages of fitting multiple-sample data sets, is "user friendly," can fit large energy regions in one run, was written specifically for this problem, uses cross-section equations identical to those of processing codes, has appropriate truncation terms, and employs resolution functions tailored for the ^{238}U resolved-resonance region. Its major disadvantages are its non-treatment of transmission correlations over sample thickness and its basic non-Bayesian character. SAMMY, on the other hand, is a full Bayesian code; however, it seems to be relatively cumbersome. Presently, people fit approximately 125 data points at a time. From 880 eV to 10,000 eV the ORNL 150-m data set contains 80,000 data points (20,000 energies $\times$ 4 sample thicknesses) and shows over 700 resonances. It is not a viable option to analyze this data set a few hundred points at a time.

Consequently, SIOB and other programs should be further developed to (1) correctly account for the transmission correlations over sample thickness and (2) to be Bayesian in the input parameters. The essential feature of an effectively diagonal or easily invertible transmission covariance matrix must be retained. All the non-diagonal covariance in the transmission data could be expressed in terms of systematic uncertainties in global parameters of the fitting function. In SIOB these are presently treated as least-squares fitting parameters with no prior treatment of uncertainties. A prior treatment of the uncertainties on these global parameters may not be that difficult and would combine the best features of SIOB with the best features of SAMMY. The effective temperature should be made a variable. With such a code only the parameter matrix would require general inversion, so thousands of data points would be fit in one run.

10.2 SHORT-TERM (ANALYSIS) RECOMMENDATIONS

In the short term, the existing data require reanalyses. The ORNL 150-m data should be reanalyzed from 0.88 to 10.0 keV in a consistent fashion, using an updated version of SIOB or a similar code. These data contain over 80,000 data points and show over 700 resonances, so a single computer run is probably not possible. Consequently, a complete, consistent, and conceptually correct fit will probably require a two-step process. The first step would consist of fitting the transmission piecewise over energy with the important global and resonance parameters as variables. The second step would consist of fitting all the piecewise first-step output covariance matrices with a code such as Bayes.[17] In this second step all the global and resonance parameters would be fitted to first-step output covariance matrices. This step would introduce the correlations between the lowest and highest energy neutron widths and give neutron widths consistent with a common set of global parameters. In principle, the results would be the same as if the entire data set had been fit in one run.[18] If necessary, the prior uncertainties could also be introduced in the second step.

There are several important questions concerning the treatment of the global parameters as a function of energy in such a fit. How would the resolution parameters be treated as a function of energy? How would the effective radius be treated? Presently, the effective radius increases with energy, partly because, on the average, it also accounts for the missed p-wave resonances.[2] From lower-energy data the effective radius was determined to be 9.44 ± 0.05 fm.[19] Perhaps the radius should be fixed at this low-energy value and a smooth cross section added at higher energies. The S parameter could probably be set to zero for the piecewise fits without affecting the results.

The input transmission data files and parameter files exist for the 31 fitted SIOB energy pieces of the ORNL data from 0.8 to 10.0 keV so this reanalysis would not be difficult. Results from the 15 energy pieces from 0.880 to 4.00 keV have been published.[2] The region from 4 to 6 keV has been fit with eight energy pieces and the results have been published.[20] For these fits the resolution function was treated correctly but the excess-background and normalization corrections were fixed at zero. In addition, the neutron width uncertainties were significantly overestimated. The region from 6 to 10 keV has been fit with eight energy pieces, yielding parameters for 230 resonances. A complete reanalysis of the entire data set should give consistent and conceptually correct neutron widths accurate to ±2% below 4 keV and ±5% below 10 keV.

The CBNM (1 to 4 keV) and JAERI (1 to 3 keV) transmission data could also be fit in a similar two-step fashion and the results from the three measurements combined. In such a combination, the ORNL neutron widths would greatly outweigh those of CBNM and JAERI. However, the three sets of neutron widths would probably demonstrate systematic deviations of less than 2 to 4% over all energies. In a minimum effort, the CBNM and JAERI data could be used to verify the ORNL results by calculating and comparing the former transmissions from resonance parameters from the latter transmissions.

10.3 LONG-TERM (MEASUREMENT) RECOMMENDATIONS

Long-term recommendations largely deal with new measurements. New transmission measurements with the accuracy of the existing CBNM and JAERI measurements will not significantly change the present data base. New transmission measurements with either cooled or room-temperature samples with the same instrumental resolution as the existing ORNL results would at least verify the existing data base. Figure 12 compares raw time-of-flight spectra from identical 155-m measurements through a 0.012 b^{-1} sample. These data from 1975 were not reduced and analyzed. One spectrum (histogram) is from the sample at room temperature and the other spectrum (data points with error bars) is from the sample cooled to liquid nitrogen. At these energies the difference in total resolution is small, since both cooled samples and improved instrumental resolution are required to significantly reduce the total resolution. The calculated difference in resolution between the two spectra is ~20%. With increasing energy the resolution gains with cooling are reduced since the instrumental resolution increasingly dominates the Doppler broadening. To significantly improve the resolution of the transmission data base, a 300- to 400-meter measurement with cooled samples and short bursts (<5 ns) would have to be made with a good detector. Such a measurement is recommended with 0.15, 0.05, and 0.017 b^{-1} samples.

In addition, there is a pressing need for a high-resolution capture measurements, particularly for analyses above 4 keV. The major confusion in analyzing thick-sample transmission data is the location of small resonances. Small resonances are best observed in capture. Also, any measurement which can further separate the small resonances into p-wave and s-wave population is of significant value. In a practical sense, recommendations for new measurements must be made in light of the required accuracy for neutron widths. The existing data can give neutron widths below 4 keV from at least two measurements with a systematic difference of less than or equal to 4%.

11. SUMMARY

SIOB FITS TO THE ORNL, CBNM, AND JAERI TRANSMISSIONS

1. If the three data sets are analyzed by the same shape-fitting code and if the data are allowed to choose their own resolution-function parameters, then much of the neutron width discrepancy is removed.
2. The best-fit resolution functions are highly asymmetric and wider than one would have initially assumed. The JAERI resolution function is very wide.
3. The CBNM samples appear to have been 15 to 20°K warmer than the JAERI sample.
4. There is substantial confusion between the resolution-function tails and excess-background corrections with fits to the CBNM and JAERI data. This confusion does not exist with the ORNL data. Variable excess-background corrections for the CBNM and JAERI data seem to converge to unrealistic values, giving larger and more discrepant neutron widths.
5. With no excess-background corrections, the CBNM neutron widths are on the average −2.0%, +1.7%, and 4.1% larger than those of ORNL for regions 1, 2, and 3, respectively. The corresponding deviations for the JAERI neutron widths are −8.8%, +0.4%, and +0.6%. The −8% JAERI region-1 discrepancy is probably a background problem. The origin of the +4% CBNM region-3 discrepancy is not clearly understood.
6. With reanalysis and reasonable assumptions, the systematic neutron-width discrepancy between the three measurements would be less than 2 to 4%.
7. With reanalysis, the ORNL data would provide neutron widths individually accurate to ±2% below 4 keV and ±5% below 10 keV.
8. Unless the neutron-width accuracy requirement is less than 3% below 4 keV, the present data base is probably sufficient.
9. The neutron widths are larger than those contained in any existing evaluation.

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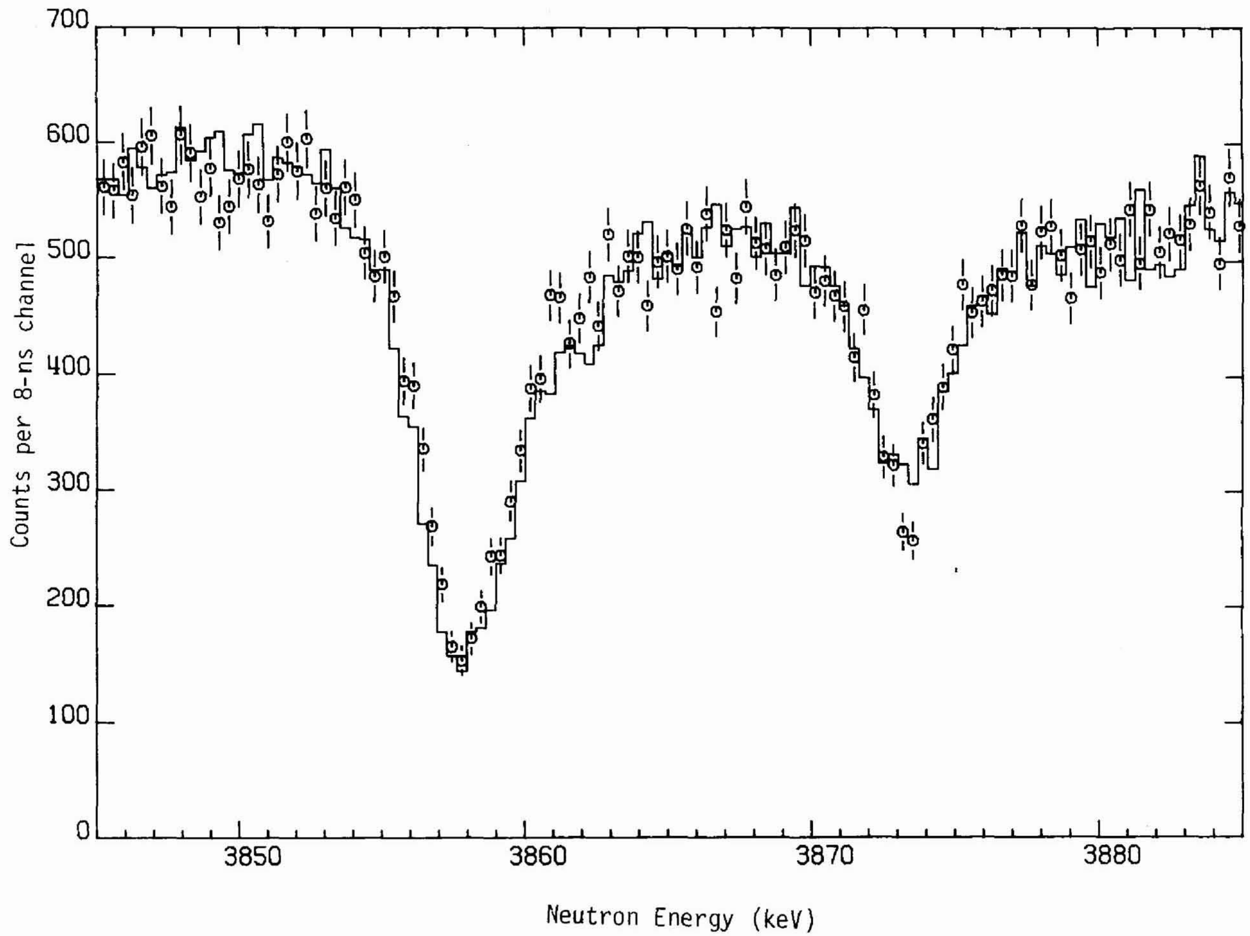

Fig. 12. Comparison of 155-m measured time-of-flight spectra through a 0.012 b^{-1} ^{238}U sample at room temperature (histogram) and liquid-nitrogen temperature (data points with error bars). The difference in resolution is calculated to be ~20%.

10. Recommendations for future work should be made in light of the accuracy requirements for these data.

CODE RECOMMENDATIONS

11. SIOB and other shape programs should be developed to correctly account for transmission correlations over sample thickness. All other systematic problems should be expressed as uncertainties on fitting function parameters so that a "user friendly" Bayesian code results which is capable of fitting thousands of data points in a single run. That is, the covariance matrix of the input transmission data should remain effectively diagonal for a general use code.

SHORT-TERM (ANALYSIS) RECOMMENDATIONS

12. The three data sets should be reanalyzed in a consistent, complete, and conceptually correct fashion. This would probably require two steps. First, the data would have to be fitted piecewise over energy with all the important global parameters variable. Secondly, the neutron widths should be reconciled to constant or smoothly varying global parameters by a Bayesian fit of the resulting parameters to the first-step output covariance matrices. As a minimum effort, the ORNL data should be so analyzed from 0.88 to 10.0 keV and the resulting neutron widths tested for consistency with the JAERI and CBNM data. If the three data sets were all reanalyzed and combined, the much smaller uncertainties of the ORNL widths would result in neutron widths probably within 1% of the stand-alone results.

LONG-TERM (MEASUREMENT) RECOMMENDATIONS

13. New transmission measurements with the accuracy of the existing CBNM and JAERI data could not significantly alter the present data base. New transmission measurements with the accuracy and instrumental resolution of the ORNL data with or without cooled samples would tend to do little more than verify the existing ORNL results.
14. A high resolution 100- to 200-m capture measurement is probably the most important new measurement to improve the data base.
15. A transmission measurement at 300 to 400 m with cooled samples, a good resolution detector, low background, and short burst widths through 0.15, 0.05, and 0.017 b^{-1} samples would significantly improve the data base.
16. Any measurements which better separate the small resonances into p-wave and s-wave populations is of value.

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