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A STUDY OF THE EFFECTIVE RESONANCE INTEGRAL AND DOPPLER COEFFICIENT OF U238, Th232, AND Pu240 USING THE CODE COMPLEX LUBRA

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ABSTRACT

The effective resonance integral and Doppler coefficient of U238, Th232, and Pu240 have been studied in detail using the LUBRA complex of codes. Some earlier results were used for comparison to verify the validity of the LUBRA results. Discrepancies have been explained and confidence can be placed in the results given by the LUBRA codes.

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1. INTRODUCTION

The LUBRA complex of codes (Kletzmayr 1966) was written to provide an automatic computational method for calculating resonance integrals, Doppler coefficients, and cross section data. LUBRA was also intended as a research tool to be employed in the comparison of the various resonance absorption theories.

An important step in the commissioning of a reactor code is a complete checkout of its various features to ensure the absence of any errors that may have arisen in the theory, numerical analysis, or coding. To fulfil this aim and to provide useful data, a detailed study of the effective resonance integral and Doppler coefficient was carried out for U238, Th232, and Pu240.

The approach was to compare LUBRA output with results obtained by other means. This included:

(i) verifying that the numerical results from LUBRA reproduce specific values obtained analytically,

(ii) a check of values obtained for effective resonance integrals and Doppler coefficients against previous computations, and

(iii) comparison with independent coding of those parts of LUBRA which have been incorporated into other codes.

2. FORMULAE AND NOTATION

The resonance theories incorporated into the LUBRA complex of codes have been described in detail by Kletzmayr (1966). However, the following brief outline of the formulae used in LUBRA to evaluate resonance integrals and Doppler coefficients is given for convenience.

The effective resonance integral for a single resonance at energy E_r for all models included in LUBRA is expressed by the general formula:

$$I_{eff} = \frac{\Gamma_a \sigma_o}{E_r} \, f(p) \, \beta_\lambda \, J(\theta, \beta_\lambda) \quad ,$$

and the Doppler coefficient at a particular temperature by:

$$D_c = G \, f^*(p) \, \beta_\lambda \left(\frac{\theta}{T}\right) \frac{\partial J(\theta, \beta_\lambda)}{\partial \theta} \quad ,$$

where

$$G = \frac{1}{\bar{\xi}(\sigma_M + \sigma_b)} \, \frac{\Gamma_a \sigma_o}{2 E_r} \quad ,$$

$f(p) = 1$, $f^*(p) = 1$ } for all models except the modified-λ model proposed by McKay, Keane, and Pollard (1965), in which case:

$$f(p) = \frac{2}{1 + p}$$

$$f^*(p) = \frac{2}{1 + p(1 + \ln p)}$$

with $p = \exp\left\{-I_{eff}/\bar{\xi}(\sigma_M + \sigma_b)\right\}$.

$$\beta_\lambda = \begin{cases} \dfrac{\sigma_M + \sigma_b}{\sigma_0} & \text{for the N.R. approximation,} \\[2ex] \dfrac{\sigma_M}{\sigma_0} & \text{for the N.R.I.A. model,} \\[2ex] \dfrac{\Gamma}{\Gamma_a + \lambda_0 \Gamma_n} \dfrac{\lambda_T \sigma_M}{\sigma_0} & \text{for the modified-}\lambda\text{ model, where } \lambda_0, \lambda_T \text{ are the interpolation constants for the absorber and the whole system respectively.} \end{cases}$$

$$J(\theta, \beta_\lambda) = \int_0^\infty \frac{\psi(x,\theta)}{\psi(x,\theta) + \beta_\lambda} dx$$

where $\psi(x,\theta)$ is the Doppler broadened line-shape function,

$$\left(\frac{\theta}{T}\right) \frac{\partial J(\theta,\beta_\lambda)}{\partial \theta} = \frac{32\pi k E_r \beta_\lambda}{\Gamma^2 A} \left[1 - \frac{1}{b_\lambda} - \frac{1}{2b_\lambda(1+\beta_\lambda)} \left\{ 1 + \frac{3}{4\beta_\lambda} \right\} \right]$$

for $T = 0\,^\circ K$,

and $\dfrac{\partial J(\theta,\beta_\lambda)}{\partial \theta}$ is evaluated by quadratic interpolation of J-functions for non-zero temperatures.

$$b_\lambda^2 = 1 + \frac{1}{\beta_\lambda}$$

σ_M = potential scattering cross section of the moderator per absorber nucleus,

σ_b = potential scattering cross section of the absorber nucleus,

$\bar{\xi}$ = the average energy loss for the system,

$\theta = \dfrac{\Gamma}{2} \sqrt{\dfrac{A}{kTE_r}}$,

T = temperature in degrees Kelvin,

k = Boltzmann's constant (8.61×10^{-5} eV/ °K)

A = atomic mass number of the absorber nucleus,

Γ_n = neutron scattering width of the absorber at resonance energy E_r,

Γ_γ = neutron capture width of the absorber at resonance energy E_r,

Γ_f = neutron fission width of the absorber at resonance energy E_r,

Γ_a = total neutron absorption width = $\Gamma_\gamma + \Gamma_f$,

Γ = total neutron width at resonance energy E_r,
= $\Gamma_\gamma + \Gamma_f + \Gamma_n$,

g_J = statistical spin factor of the absorber at energy E_r,

and σ_0 = peak height of the resonance,
= $2.608 \times 10^6\, \Gamma_n g_J / \Gamma E_r$.

The average Doppler coefficient for any temperature range is evaluated from:

$$D_c = \frac{1}{p} \frac{\Delta p}{\Delta T}$$

which for all models, except the modified-λ model, reduces to

$$D_c = - \frac{1}{\bar{\xi}(\sigma_M + \sigma_b)} \frac{\Delta I_{eff}}{\Delta T}$$

3. THE EFFECTIVE RESONANCE INTEGRAL OF U238

3.1 The Infinitely Dilute Resonance Integral

The parameters used for the resolved resonances of U238 were those given in BNL-325 (Hughes and Harvey 1955). These are the same data as used by Sampson and Chernick (1958) and Dresner (1956).

The infinitely dilute resonance integral was calculated by LUBRA as 266.8 barns, which is 2.4 barns higher than the value quoted by Sampson and Chernick. This may be explained by the fact that LUBRA calculates infinitely dilute resonance integrals using $\int_{E_c}^{\infty} \sigma_a \frac{dE}{E}$, where E_c is some low energy cut-off (taken as 0.4 eV), instead of the usual approximation $\frac{1}{E_r} \int_{-\infty}^{\infty} \sigma_a \, dE$.

An additional difference is due to the use in LUBRA of the asymmetric form of σ_a, which contains the factor $\sqrt{E_r/E}$.

3.2 The Effective Resonance Integral of the Resolved Resonances

A set of results given by Dresner (1956) was re-computed using LUBRA and the comparison is set out in Table 1. Except for $\sigma_p = 2000$ barns at T = 300 °K, the agreement for the resolved resonances is excellent. For this one discrepancy Dresner's value is about 10 per cent. lower than that obtained from LUBRA and, as is shown in Section 4.1, precisely the same discrepancy occurs for Th232. We have not been able to explain this difference and must rely on some other comparison for the justification of the accuracy of LUBRA.

An alternative check can be obtained from a comparison with the total effective resonance integrals tabulated by Blake (1960). Although slightly different resonance data were used, the agreement, shown in Table 2, is very good over the range of σ_p and T considered by Dresner, thus substantiating the accuracy of the LUBRA calculations. There is a slight drift in the agreement with increasing temperature, particularly at low resonance absorber concentrations, which can only be attributed to Blake's use of Roe's (1954) approximation to the J-function. An overall difference of 0.3 per cent. is due to the choice of the constant in σ_0, taken as 2.608×10^6 in LUBRA.

3.3 The Unresolved Resonance Integral

Both Dresner (1956) and Sampson and Chernick (1958) have given numerical values for the contribution to the effective resonance integral by the unresolved resonances of U238. In particular Sampson and Chernick quoted results showing the reduction produced by the statistical variation of the resonance parameters and the enhancement resulting from the contributions from higher orbital angular momentum states.

In calculating unresolved resonance integrals, Dresner approximated:

$$\int_{E_1}^{\infty} J(\theta,\beta) \frac{dE}{E}$$

by

$$\int_{\beta_1}^{\infty} J(0.1,\beta) \frac{d\beta}{\beta},$$

where $\beta_1 = \sigma_p E_1 / 2.60 \times 10^6$ and $\sigma_p = \sigma_M + \sigma_b$. These approximations are a consequence of assuming that $\Gamma_n << \Gamma_\gamma$.

On the other hand, if we assume that $\Gamma_n = \Gamma_\gamma$ for all resonances, since this is more reasonable for the important lower end of the unresolved region, then:

$$\int_{E_1}^{\infty} J(\theta,\beta) \frac{dE}{E} \doteqdot \int_{2\beta_1}^{\infty} J(0.2,\beta) \frac{d\beta}{\beta} .$$

When $E_r = 400$ eV and $\sigma_p = 2000$ barns, then $\beta_1 \doteqdot 0.33$ or $k \doteqdot 15$. Using Dresner's tables which are tabulated for values of k, where k is given by $\beta = 2^k \times 10^{-5}$, we find that:

$$J(0.1, 2^{15} \times 10^{-5}) = 4.088$$

$$J(0.2, 2^{16} \times 10^{-5}) = 2.067 ,$$

so that the assumption, $\Gamma_n = \Gamma_\gamma$, could give half the value of the integrand at the important lower end of the energy range. Again, if $\sigma_p = 20$ barns, so that $k \doteqdot 9$, we obtain from Dresner's tables:

$$J(0.1, 2^9 \times 10^{-5}) = 3.787$$

$$J(0.2, 2^{10} \times 10^{-5}) = 2.153 ,$$

showing that Dresner's assumption gives an estimate 75 per cent. higher than that obtained from $\Gamma_n = \Gamma_\gamma$.

It is worth noting that, for T = 0 °K, $J(\infty,\beta) = \frac{\pi}{2\sqrt{\beta(1+\beta)}}$ so that

$$\int_{\beta_1}^{\infty} J(\infty,\beta) \frac{d\beta}{\beta} = \pi \left(\sqrt{\frac{1+\beta_1}{\beta_1}} - 1 \right)$$

. Thus the assumption $\Gamma_n << \Gamma_\gamma$ at energy E_1 gives an estimate:

$$\left(\frac{\sqrt{(1+\beta_1)/\beta_1} - 1}{\sqrt{(1+2\beta_1)/2\beta_1} - 1} - 1 \right) \times 100$$

per cent. higher than that obtained for the assumption $\Gamma_n = \Gamma_\gamma$.

For large β_1 this expression tends in the limit to 100 per cent., while for $\beta_1 \to 0$, it tends to slightly more than 40 per cent.

The values of the unresolved resonance integral of U238 obtained by Dresner are compared with corresponding LUBRA values in Table 1. Dresner's values are roughly 30 per cent. higher for $\sigma_p = 20$ barns and 50 per cent. higher for $\sigma_p = 2000$ barns. This is consistent with the previous observations on the errors introduced by Dresner at the lower end of the range of integration.

Table 3 gives a comparison of the infinitely dilute unresolved resonance integrals as calculated by LUBRA with values quoted by Sampson and Chernick. Neglecting both the statistical variation of the resonance parameters and the contribution from higher ℓ-states, the agreement is very good. The effect of including the higher ℓ-states or the statistical variation of Γ_n^0 also gives satisfactory agreement.

4. THE EFFECTIVE RESONANCE INTEGRAL AND DOPPLER COEFFICIENT OF Th232

4.1 The Total Effective Resonance Integral

Keane, McKay, and Clancy (1959) calculated the effective resonance integrals of Th232 for a variety of moderator concentrations and temperatures using the data quoted in BNL-325 (Hughes and Harvey 1955). The values of the line-shape function $\psi(x,\theta)$ were obtained from tables compiled by Rose et al. (1954), and the numerical integrations were performed on a desk machine. The Narrow-Resonance approximation was assumed and both the contribution from higher ℓ-states and the statistical distribution of the resonance parameters were neglected in the unresolved region.

As a check on the validity of the present work, these earlier calculations were repeated by the LUBRA code. Although the same data were used differences were expected to arise because:

(i) LUBRA generates its own Doppler broadened line-shape functions, $\psi(x,\theta)$, and

(ii) the numerical integration required to evaluate each J-function, $J(\theta,\beta)$, is performed far more accurately by LUBRA with the aid of the routine of Bell, Buckler, and Pull (1963) than could be expected from a hand calculation.

A brief check of the tabulated $\psi(x,\theta)$-values against values obtained by the LUBRA routine shows that the differences between the two sets of results for the range under consideration are negligible.

A comparison of the values of the effective resonance integrals obtained from LUBRA with the values published by Keane et al. (1959) in their report E49 is given in Tables 4 and 5 and graphed in Figure 1. For low σ_M the differences between the E49 and LUBRA values, with the statistical distribution of Γ_n^o and higher ℓ-state contributions neglected, is less than 2 per cent, while for σ_M = 1000 barns the difference is approximately 0.2 per cent. The value of the constant σ_o, taken as 2.608×10^6 in LUBRA, would account for values 0.3 per cent. higher than those given in E49.

The differences are greatest for small values of θ where the tabulation of the ψ-function by Rose et al. (1954) was given for only a small set of x-values. In view of the shape of the curve $\psi/(\psi + \beta)$ we would expect the desk calculations of the J-functions to have large errors for small θ-values and small dilutions.

Inclusion of the statistical distribution of Γ_n^o and higher ℓ-state contributions lowers the contribution of the unresolved resonances to the effective resonance integral by 10 per cent. for small σ_M and by 20 per cent. for infinitely dilute systems. This suggests that the assumption made by Keane et al. (1959), that the decrease in the effective resonance integral value from the statistical variation of Γ_n^o balances the contribution from $\ell > 0$ states is not valid. This assumption was made on the basis of the results given by Sampson and Chernick (1958), where it was approximately valid for U238. However, it was not realized at the time that the relative contributions from higher orbital angular momentum states and the statistical distribution of Γ_n^o depended on the energy of the last resolved resonance. It is now evident that, since the contribution from higher ℓ-states is only important at high energies, it is effectively independent of the energy of the last resolved resonance, while the reduction due to the statistical variation of the unresolved resonance parameters is roughly proportional to the total unresolved integral.

A comparison of results obtained from LUBRA with those quoted by Dresner (1956) is presented in Table 6. For the resolved resonances the agreement is excellent, as it was for U238, except for σ_p = 2000 barns at T = 300 °K, where Dresner's value is 10 per cent. lower.

For the unresolved resonances Table 6 shows a marked difference between the LUBRA values and those given by Dresner. This point was considered in detail in Section 3.3, where similar results for U238 were investigated.

Comparison with Blake's values for the total effective resonance integral of Th232, set out in Table 7, shows agreement similar to that obtained for U238.

4.2 The Doppler Coefficient of the 22 eV Resonance

The Doppler coefficient of the 22 eV resonance of Th232 was evaluated for Th/Be systems at several temperatures using the standard A.A.E.C. library data (Doherty 1964) in the N.R. and modified-λ formulae. As can be seen from Table 8 and Figure 2, the N.R. approximation has several turning points. The T = 0 °K curve has a minimum at $\sigma_M \doteqdot 8.5 \times 10^2$ barns and a maximum at $\sigma_M \doteqdot 30$ barns, from which it descends rapidly to a lower limit determined when $\sigma_M = 0$.

As the temperature increases, the minimum shifts towards lower σ_M-values and becomes broader. At T = 300 °K, the minimum and maximum exhibited so strongly at T = 0 °K, no longer exist.

The curves shown in Figure 3, based on the modified-λ model, have a single minimum only and approach zero both at low and at high moderator scattering.

The observed behaviour of the curves can be partly explained using the results of a study of the minimum Doppler coefficient by Keane and Horner (1966). They showed that for T = 0 °K the minimum value occurs at $\beta \doteqdot 0.1$, and that with increasing temperature there is a decrease of both the magnitude of the minimum and the value of β for which this minimum occurs. Since the value of σ_0 for the 22 eV resonance of Th232 is 9.13×10^5 barns the observed value of σ_M at the minimum of the T = 0 °K curves corresponds closely to $\beta = 0.1$.

The slight decrease for the N.R. model in the value of β below 0.1 and in the maximum obtained for small dilutions is caused by variations in $\bar{\xi}$. To obtain an estimate of the position of the maximum for the T = 0 °K curve, we have for the N.R. approximation:

$$D_c \propto \frac{1}{\bar{\xi}} \frac{\partial J(\theta,\beta)}{\partial \theta},$$

where $\bar{\xi} \doteqdot \dfrac{\xi_{Be}\,\sigma_M}{\sigma_M + \sigma_b}$, since $\xi_{Th} << \xi_{Be}$.

Since $\dfrac{\partial J(\theta,\beta)}{\partial \theta} \doteqdot \dfrac{3}{4}\pi\sqrt{\beta}$ for small β, we then have

$$D_c \propto \frac{(\sigma_M + \sigma_b)^{\frac{3}{2}}}{\sigma_M},$$

The position of the turning point for small σ_M is then found from:

$$\frac{\partial D_c}{\partial \sigma_M} = 0 \qquad \text{or} \qquad \sigma_M \doteqdot 2\,\sigma_b .$$

This estimate is in close agreement with the value of $\sigma_M \doteqdot 30$ barns obtained from the graph in Figure 2.

4.3 The Effect of Data on the Doppler Coefficient

The Doppler coefficient is sensitive both to variations in the resonance parameters and to the model used for the calculation of resonance absorption.

To obtain an idea of the sensitivity to data the Doppler coefficient was calculated from the N.R. formula for the lowest resonance of Th232 at T = 0 °K for a moderator scattering cross section of 100 barns per thorium atom, using three sets of data:

(i) E_r = 22.0 eV
Γ_n = 2×10^{-3} eV
Γ_γ = 3×10^{-2} eV
} BNL-325 (Hughes and Harvey 1955) data

(ii) E_r = 21.84 eV
Γ_n = 1.78×10^{-3} eV
Γ_γ = 2.15×10^{-2} eV
} A.A.E.C. library data (Doherty 1964)

(iii) E_r = 21.78 eV
Γ_n = 2×10^{-3} eV
Γ_γ = 2.5×10^{-2} eV
} proposed replacement for the A.A.E.C. data.

The N.R. values of the Doppler coefficient obtained for each set of data were respectively:

(i) -9.71×10^{-5} ,

(ii) -12.27×10^{-5} ,

(iii) -10.71×10^{-5} .

Differences of up to 20 per cent. in the Doppler coefficient value for the lowest resolved resonance of Th232 are thus seen to arise from small variations in the resonance parameters.

A difference of 30 per cent. was found in the total resolved N.R. Doppler coefficient caused by variations in the resolved resonance data. The results for Th/Be systems with σ_M = 100 barns at T = 0 °K were:

(i) -9.26×10^{-4} with the BNL-325 (Hughes and Harvey 1955) data, and

(ii) -1.20×10^{-3} with the A.A.E.C. library data.

5. THE EFFECTIVE RESONANCE INTEGRAL AND DOPPLER COEFFICIENT OF Pu240

5.1 The Effective Resonance Integral for Heterogeneous Systems

McKay (Unpublished) calculated the increase in the effective resonance integrals per U238 atom, for U238 rods containing 0.04 per cent. Pu240. These calculations were repeated using the LUBRA code and the comparison is shown in Table 9.

In treating heterogeneous systems McKay used a potential scattering per absorber atom given by $\sigma_b + (1/N\bar{\ell})$, where σ_b is the scattering cross section of the material in the rod per Pu240 atom, N is the number of absorber atoms/cm^3 of rod, and $\bar{\ell}$ the mean free path, for a cylindrical rod, is equal to its diameter.

Using LUBRA this problem of a rod in an infinite isotropic neutron bath was simulated by taking a large value (10^8 barns) for the external moderator scattering cross section. Thus the expression $\sigma_M/(1+N\bar{\ell}\sigma_M)$ is very nearly $1/N\bar{\ell}$.

A difference of between 1½ and 3 per cent. in the values was explained by McKay (1961) as due to his method of interpolating the J-function tables.

5.2 The Total Effective Resonance Integral for Homogeneous Systems

Table 10 shows a comparison of LUBRA values for the total effective resonance integral (resolved + unresolved + 1/v contribution) of Pu240 with results tabulated by Blake (1960). The two sets of values agree to the same extent as was found for the U238 and Th232 results.

5.3 The Doppler Coefficient of the 1 eV Resonance

One difficulty which occurs for Pu240 results from the fact that the 1 eV resonance is so near the thermal region and hence influenced by spectrum shift. This will affect the temperature coefficient of the resonance but not the Doppler coefficient which is only produced by the lowering and broadening of the resonance contour. In most calculations it has been found (Pollard, Private Communication) that the effect of the spectrum shift on the temperature coefficient of the 1 eV resonance can be allowed for by taking the first term in the asymptotic expansion of the flux, namely $1 + (2T/E_r)$.

Tables 11 and 12 and Figures 4 and 5 give the Doppler coefficient of the 1 eV resonance of Pu240 for the N.R. and modified -λ models.

The points of interest are:

(i) The minimum of the N.R. curve at T = 0 °K lies at $\sigma_M \doteqdot 1.60 \times 10^4$ barns. Since the peak height of the resonance is 1.61×10^5 barns, this gives $\beta \doteqdot 0.1$, which is in agreement with the result by Keane and Horner (1966).

(ii) The minimum value of the modified -λ curve occurs at about the same point but is nearly 20 per cent. higher.

(iii) For dilutions of the order of 1000 barns the modified -λ model gives values more than 60 per cent. lower than the N.R. approximation.

Table 13 shows, for each temperature used in Table 11, the value of β for which the minimum Doppler coefficient occurs and the ratio of the minimum value to that for T = 0 °K. For each temperature this value of β was obtained from the least squares fit of a quadratic to the five points which can be seen from Table 11 to straddle the minimum. The agreement between the values obtained by interpolating the table of Keane and Horner (1966) with those from Table 11 provides a valuable check on the accuracy of the LUBRA results. The slightly lower values of β obtained from LUBRA can be attributed to the variation of ξ with dilution which has been taken into account in the LUBRA calculations but not by Keane and Horner.

Figure 6 shows the average Doppler coefficients, calculated from effective resonance integrals at T = 0(300)1500 °K, superimposed on the curves evaluated from the point formulae. For all models the agreement is as expected hence verifying the consistency of the two different methods of calculating Doppler coefficients.

6. COMPARISON OF LUBRA WITH GYMEA

The GYMEA code written by Pollard and Robinson (1966) uses the approximate J-function routine RESJ (Doherty 1963) to calculate resonance absorption as a function of both temperature and dilution. The theory incorporated into RESJ essentially gives a curve of best fit for the values of the J-function tabulated by Bell, Buckler, and Pull (1963).

Effective resonance integrals obtained from LUBRA and GYMEA were compared for U238, Th232, and Pu240 at T = 0 °K and 300 °K using the N.R. approximation. The results of this comparison are set out in Tables 14, 15, and 16. Agreement at T = 0 °K is perfect, as it should be, and good agreement is obtained at T = 300 °K.

Table 17 shows the average Doppler coefficients for the three absorbers in question calculated by LUBRA from the modified -λ model over the temperature range 0–1500 °K in steps of 300 degrees. The differences between the two sets of results are less than 10 per cent.

7. CONCLUSIONS

The series of calculations needed to perform this checkout involved LUBRA 1, LUBRA 2, and LUBRA 3. Consistent results were obtained and it can be stated with confidence that the code calculates effective resonance integrals and Doppler coefficients accurately in accordance with the formulae incorporated into LUBRA.

In the course of this checkout, which was run in conjunction with the commissioning of the LUBRA complex of codes, some errors were found and rectified.

Analytical check points suggested by the LUBRA output have been pursued both in this report and elsewhere (Keane and Horner 1966), and in all cases the numerical results have been verified. Differences between the values from LUBRA and earlier calculations have been explained and attributed to different numerical methods. In all instances the LUBRA results are held to be more accurate.

The sensitivity of the Doppler coefficient to data and model was also studied. While the choice of model does not introduce any significant changes for U238 and Th232 for realistic dilutions, differences of up to 60 per cent. result from the choice of model for Pu240. This is to be expected in view of the inadequacy of the N.R. model for the 1 eV resonance of Pu240. Two different sets of resonance parameters for Th232 gave a 30 per cent. change in the value of the total resolved Doppler coefficient.

The comparison with GYMEA was far more consistent than anticipated and gives a reassuring check on the validity of some of the approximate methods incorporated into this multipurpose code.

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TABLE 1

COMPARISON OF THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF U238 OBTAINED FROM LUBRA, USING THE BNL-325 (1955) DATA, WITH DRESNER'S (1956) RESULTS

Temperature (°K)	$\sigma_M + \sigma_b$ (barns)	LUBRA Values		Dresner's Results	
		resolved	unresolved*	resolved	unresolved
0	20	7.73	1.27	7.9	1.7
	200	24.28	3.48	24.0	4.8
	2000	73.32	7.18	74.0	11.0
300	20	8.05	2.18	8.1	3.0
	80	16.75	4.22	17.0	6.6
	200	27.61	5.90	27.0	9.4
	2000	96.35	9.12	86.0	12.0

* the unresolved LUBRA values include neither the statistical variation of Γ_n^o nor higher ℓ-state contributions

TABLE 2

COMPARISON OF LUBRA RESULTS FOR THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF U238 WITH VALUES QUOTED BY BLAKE (1960) USING BLAKE'S RESONANCE PARAMETERS

$\sigma_M + \sigma_b$ (barns)	T = 0 °K		T = 300 °K		T = 600 °K		T = 1000 °K		T = 3000 °K	
	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE
20	10.14	10.13	11.56	11.45	12.18	12.00	12.77	12.50	14.47	13.98
50	15.16	15.15	17.72	17.63	18.78	18.59	19.82	19.49	23.04	22.15
100	20.73	20.71	24.59	24.52	26.25	26.00	27.90	27.42	33.19	31.76
300	34.25	34.21	41.69	41.55	45.25	44.73	48.85	47.88	60.20	57.81
600	46.96	46.90	58.52	58.22	64.29	63.50	69.99	70.84	86.99	84.41
1000	59.05	58.98	75.13	74.68	83.06	82.10	90.61	92.12	111.95	109.60
2000	79.91	79.80	104.21	103.63	115.29	114.31	125.20	127.72	150.59	148.87
5000	116.12	115.94	152.11	151.55	165.47	164.72	176.26	179.36	200.20	199.19
10,000	149.00	148.75	189.29	188.78	201.48	200.88	210.59	213.15	228.89	228.11
100,000	242.94	242.37	258.92	258.29	261.71	261.06	263.52	263.44	266.59	265.81
∞	273.13	271.16	273.13	271.16	273.13	271.16	273.13	271.16	273.13	271.16

TABLE 3

THE EFFECT OF THE STATISTICAL VARIATION OF Γ_n^o AND HIGHER ℓ-STATE CONTRIBUTIONS AS OBTAINED FROM LUBRA FOR U238 COMPARED WITH RESULTS QUOTED BY SAMPSON AND CHERNICK (1958)

	Infinitely Dilute Unresolved Resonance Integral	
	LUBRA	Sampson and Chernick
Both the statistical variation of Γ_n^o and higher ℓ-state contributions neglected	9.86	10.0
Effect of higher ℓ-state contributions only included	12.38	13.1
Effect of including the statistical variation of Γ_n^o only	6.82	7.0
Both the statistical variation of Γ_n^o and higher ℓ-state contributions included	8.56	–

TABLE 4

COMPARISON OF THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF Th232 AT T = 0°K, AS OBTAINED FROM THE NARROW RESONANCE AND MODIFIED-λ MODELS USING LUBRA, WITH RESULTS BY KEANE ET AL. (1959)

σ_M (barns)	Keane et al.	LUBRA results N.R.					LUBRA modified-λ results	
		resolved	unresolved*	unresolved**	total*	total**	resolved	total***
10	5.39	3.90	1.54	1.37	5.44	5.27	3.49	4.76
20	6.40	4.68	1.82	1.61	6.50	6.29	4.63	6.24
50	8.77	6.47	2.45	2.15	8.92	8.62	6.82	8.97
80	10.69	7.86	2.90	2.53	10.76	10.39	8.36	10.89
100	11.73	8.65	3.16	2.74	11.81	11.39	9.22	11.96
200	15.61	11.81	4.09	3.50	15.90	15.31	12.53	16.03
500	23.20	18.01	5.65	4.74	23.66	22.75	18.82	23.56
800	28.55	22.29	6.54	5.44	28.83	27.73	23.12	28.56
1000	31.52	24.61	6.97	5.77	31.58	30.38	25.44	31.21
∞		80.02	11.30	9.09	91.32	89.11		

* unresolved resonance integral neglecting both statistical distribution of Γ_n^o and higher ℓ-state contributions

** unresolved resonance integral including both the statistical distribution of Γ_n^o and higher ℓ-state contributions

*** includes N.R. values for the unresolved region as given by **

TABLE 5

COMPARISON OF THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF Th232 AT T = 300°K, AS OBTAINED FROM THE NARROW RESONANCE AND MODIFIED –λ MODELS USING LUBRA, WITH RESULTS BY KEANE ET AL. (1959)

σ_M (barns)	Keane et al.	LUBRA N.R. results					LUBRA modified λ–results	
		resolved	unresolved*	unresolved**	total*	total**	resolved	total***
10	7.08	4.37	2.85	2.60	7.22	6.97	3.87	6.47
20	8.60	5.39	4.50	3.02	9.89	8.41	5.31	8.33
50	12.24	7.91	4.69	3.87	12.60	11.78	8.35	11.22
80	15.22	10.00	5.45	4.40	15.45	14.40	10.69	15.09
100	16.90	11.24	5.89	4.71	17.13	15.95	12.05	16.76
200	23.36	16.36	7.22	5.65	23.58	22.01	17.50	23.15
500	35.39	26.59	8.89	6.89	35.48	33.48	28.03	34.92
800	42.12	33.30	9.55	7.45	42.85	40.75	34.79	42.24
1000	46.75	36.74	9.88	7.70	46.62	44.44	38.22	45.92
∞		80.02	11.30	9.09	91.32	89.11		

*, **, *** } are as defined for Table 4 (for T = 0°K)

TABLE 6

COMPARISON OF THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF Th232 OBTAINED FROM LUBRA, USING THE BNL–325 (1955) DATA, WITH DRESNER'S (1956) RESULTS

Temperature (°K)	$\sigma_M + \sigma_b$ (barns)	LUBRA Values		Dresner's Results	
		resolved	unresolved*	resolved	unresolved
0	20	3.67	1.54	3.7	2.2
	200	11.48	4.69	12.0	6.3
	2000	32.93	8.25	33.0	14.0
300	20	4.08	3.22	4.0	4.0
	80	9.18	6.09	8.9	8.6
	200	15.82	8.33	15.0	12.0
	2000	47.76	10.54	42.0	20.0

* the unresolved LUBRA values include neither the statistical variation of Γ_n^o nor higher ℓ–state contributions

TABLE 7

COMPARISON OF LUBRA RESULTS FOR THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF Th232 WITH VALUES QUOTED BY BLAKE (1960) USING BLAKE'S RESONANCE PARAMETERS

$\sigma_M + \sigma_b$ (barns)	T = 0°K		T = 300°K		T = 600°K		T = 1000°K		T = 3000°K	
	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE
20	9.86	9.86	11.70	11.56	12.60	12.32	13.49	13.05	16.02	15.25
50	13.46	13.45	16.96	16.81	18.57	18.23	20.12	19.57	24.47	23.47
100	17.31	17.29	22.77	22.65	25.16	24.82	27.37	26.82	33.45	32.40
300	26.30	26.26	36.39	36.32	40.24	39.98	43.61	43.17	52.23	51.41
600	34.30	34.26	47.94	47.86	52.58	52.35	56.47	56.11	65.76	65.16
1000	41.51	41.45	57.56	57.41	62.49	62.24	66.46	66.14	75.48	75.02
2000	52.91	52.83	70.97	70.73	75.71	75.45	79.33	79.05	86.94	86.61
5000	69.62	69.50	86.56	86.29	90.14	89.89	92.68	92.44	97.54	97.29
10,000	81.65	81.49	95.14	94.89	97.59	97.36	99.25	99.03	102.26	102.02
100,000	103.75	103.49	106.35	106.12	106.73	106.48	106.97	106.71	107.36	107.08
∞	108.21	107.71	108.21	107.71	108.21	107.71	108.21	107.71	108.21	107.71

TABLE 8

THE DOPPLER COEFFICIENT OF THE 22 eV RESONANCE OF Th232 AT T = 0°K AND 300°K, USING THE NARROW RESONANCE AND MODIFIED-λ MODELS WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	$-D_c \times 10^5$ at T = 0°K		$-D_c \times 10^5$ at T = 300°K	
	N.R.	modified λ	N.R.	modified λ
1	41.67	1.46	41.58	1.58
2	27.88	2.37	27.53	2.60
3	21.97	3.04	21.48	3.33
4	18.72	3.57	18.12	3.90
5	16.68	4.00	15.98	4.35
6	15.29	4.38	14.51	4.72
7	14.30	4.72	13.43	5.03
8	13.55	5.01	12.61	5.29
9	12.98	5.28	11.96	5.53
10	12.54	5.53	11.44	5.72
20	10.83	7.31	9.04	6.80
30	10.62	8.47	8.18	7.16
40	10.75	9.34	7.71	7.26
50	10.97	10.04	7.38	7.25
60	11.24	10.63	7.13	7.18
70	11.51	11.13	6.91	7.09
80	11.77	11.58	6.72	6.97
90	12.03	11.97	6.55	6.85
100	12.27	12.32	6.40	6.73
200	14.14	14.67	5.24	5.59
300	15.27	15.89	4.44	4.72
400	15.98	16.62	3.84	4.06
500	16.43	17.06	3.37	3.55
600	16.71	17.32	2.99	3.13
700	16.87	17.45	2.67	2.79
800	16.93	17.48	2.41	2.51
900	16.93	17.46	2.18	2.27
1000	16.88	17.38	1.99	2.06
2000	15.21	15.52	0.95	0.97
3000	13.17	13.37	0.56	0.57
4000	11.37	11.51	0.37	0.37
5000	9.86	9.96	0.26	0.26
6000	8.61	8.69	0.20	0.20
7000	7.58	7.63	0.15	0.15
8000	6.71	6.75	0.12	0.12
9000	5.98	6.02	0.10	0.10
10,000	5.37	5.39	0.08	0.08
50,000	0.54	0.54	0.004	0.004
100,000	0.16	0.16	0.001	0.001

TABLE 9

COMPARISON OF LUBRA WITH McKAY'S (UNPUBLISHED) VALUES FOR THE EFFECTIVE RESONANCE INTEGRAL OF HETEROGENEOUS Pu240 SYSTEMS

Radius of Rod (cm)	Contribution from	T = 300 °K		T = 600 °K		T = 900 °K		T = 1200 °K	
		LUBRA	McKay	LUBRA	McKay	LUBRA	McKay	LUBRA	McKay
0.71	1.054 eV res.	1.809	1.866	1.872	1.917	1.923	1.957	1.964	1.998
	others	0.065	0.067	0.065	0.067	0.066	0.067	0.066	0.067
	total	1.874	1.933	1.937	1.984	1.989	2.024	2.030	2.065
1.46	1.054 eV res.	1.573	1.625	1.630	1.669	1.677	1.708	1.716	1.744
	others	0.064	0.066	0.065	0.066	0.065	0.067	0.065	0.067
	total	1.637	1.691	1.695	1.735	1.742	1.775	1.781	1.811
2.21	1.054 eV res.	1.477	1.524	1.531	1.566	1.575	1.601	1.613	1.636
	others	0.064	0.066	0.064	0.066	0.065	0.066	0.065	0.067
	total	1.541	1.590	1.595	1.632	1.640	1.667	1.678	1.703

TABLE 10

COMPARISON OF LUBRA RESULTS FOR THE TOTAL EFFECTIVE RESONANCE INTEGRAL OF Pu240 WITH VALUES QUOTED BY BLAKE (1960)

$\sigma_M + \sigma_b$ (barns)	T = 0 °K		T = 300 °K		T = 600 °K		T = 1000 °K		T = 3000 °K	
	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE	LUBRA	BLAKE
20	159.01	158.9	160.95	160.7	162.02	161.6	163.12	162.5	166.62	165.3
50	244.21	244.0	248.20	247.9	250.28	249.7	252.35	251.5	258.74	256.9
100	327.40	327.1	333.99	333.6	337.24	336.6	340.41	339.4	349.93	348.0
300	506.03	505.6	519.40	519.1	525.36	524.9	531.01	530.4	547.97	546.6
600	665.96	665.3	685.55	685.4	693.91	693.7	701.89	701.7	727.19	726.3
1000	819.45	818.6	844.70	844.5	855.46	855.5	866.03	866.2	902.06	901.4
2000	1094.31	1093.1	1129.14	1128.7	1145.16	1145.3	1162.08	1162.6	1226.00	1223.9
5000	1620.33	1618.3	1675.34	1674.5	1707.44	1707.6	1744.29	1744.6	1890.30	1883.8
10,000	2184.33	2181.5	2268.92	2267.8	2327.23	2327.1	2394.70	2394.0	2650.25	2639.5
100,000	5285.43	5270.2	5561.37	5552.9	5739.71	5730.5	5912.42	5901.9	6384.59	6369.9
∞	8534.7	8505.9	8534.7	8505.9	8534.7	8505.9	8534.7	8505.9	8534.7	8505.9

TABLE 11

THE DOPPLER COEFFICIENT OF THE 1 eV RESONANCE OF Pu240 AS A FUNCTION OF MODERATOR SCATTERING PER Pu240 ATOM, USING THE NARROW RESONANCE APPROXIMATION WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	$-D_c \times 10^5$ at					
	T = 0°K	T = 300°K	T = 600°K	T = 900°K	T = 1200°K	T = 1500°K
1×10^3	5.42	5.34	5.31	5.27	5.23	5.19
2 "	6.93	6.72	6.57	6.44	6.32	6.21
3 "	7.88	7.50	7.24	7.02	6.82	6.64
4 "	8.54	8.00	7.63	7.33	7.06	6.81
5 "	9.02	8.33	7.86	7.48	7.15	6.86
6 "	9.39	8.54	7.99	7.54	7.15	6.83
7 "	9.67	8.68	8.04	7.53	7.11	6.74
8 "	9.89	8.77	8.05	7.49	7.03	6.64
9 "	10.07	8.81	8.02	7.42	6.93	6.52
1×10^4	10.20	8.82	7.97	7.33	6.81	6.38
1.2 "	10.37	8.77	7.82	7.12	6.56	6.10
1.3 "	10.42	8.72	7.72	7.00	6.43	5.96
1.5 "	10.47	8.59	7.52	6.75	6.16	5.68
1.75 "	10.46	8.39	7.25	6.45	5.84	5.35
2 "	10.40	8.16	6.96	6.14	5.52	5.04
3 "	9.86	7.19	5.90	5.07	4.46	4.00
5 "	8.43	5.53	4.31	3.57	3.06	2.69
7 "	7.14	4.34	3.27	2.64	2.23	1.93
1×10^5	5.63	3.16	2.29	1.81	1.50	1.28
2 "	2.92	1.41	0.96	0.73	0.58	0.49
3 "	1.78	0.79	0.52	0.39	0.31	0.26
5 "	0.85	0.35	0.23	0.17	0.13	0.11
7 "	0.50	0.20	0.13	0.09	0.07	0.06
1×10^6	0.27	0.11	0.07	0.05	0.04	0.03

TABLE 12

THE DOPPLER COEFFICIENT OF THE 1 eV RESONANCE OF Pu240 AS A FUNCTION OF MODERATOR SCATTERING PER Pu240 ATOM, USING THE MODIFIED-λ MODEL WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	$-D_c \times 10^5$ at					
	T = 0°K	T = 300°K	T = 600°K	T = 900°K	T = 1200°K	T = 1500°K
1 x 10^3	2.16	2.16	2.17	2.16	2.17	2.17
2 "	3.74	3.71	3.70	3.68	3.67	3.66
3 "	5.26	5.17	5.11	5.06	5.02	4.97
4 "	6.61	6.42	6.30	6.19	6.10	6.00
5 "	7.75	7.45	7.24	7.07	6.91	6.76
6 "	8.70	8.26	7.97	7.72	7.49	7.29
7 "	9.48	8.89	8.51	8.19	7.90	7.65
8 "	10.12	9.39	8.91	8.52	8.18	7.88
1 x 10^4	11.07	10.05	9.40	8.87	8.44	8.06
1.2 "	11.71	10.41	9.60	8.98	8.46	8.02
1.3 "	11.94	10.51	9.63	8.96	8.41	7.95
1.5 "	12.28	10.60	9.60	8.84	8.24	7.74
1.75 "	12.51	10.56	9.43	8.60	7.95	7.42
2 "	12.60	10.41	9.17	8.29	7.61	7.06
2.2 "	12.60	10.24	8.94	8.03	7.33	6.77
2.5 "	12.51	9.94	8.57	7.62	6.91	6.34
3 "	12.22	9.37	7.92	6.95	6.23	5.67
5 "	10.45	7.17	5.72	4.82	4.20	3.72
7 "	8.75	5.53	4.25	3.49	2.97	2.59
1 x 10^5	6.77	3.92	2.89	2.31	1.92	1.65
2 "	3.37	1.65	1.14	0.87	0.70	0.58
3 "	2.00	0.90	0.60	0.45	0.36	0.30
5 "	0.94	0.39	0.25	0.18	0.14	0.12
7 "	0.54	0.22	0.14	0.10	0.08	0.06
1 x 10^6	0.29	0.11	0.07	0.05	0.04	0.03

TABLE 13

COMPARISON OF MINIMUM DOPPLER COEFFICIENTS AS OBTAINED FROM LUBRA WITH VALUES TABULATED BY KEANE AND HORNER (1966)

T ($^\circ$K)	$t = \frac{4kTE_r}{\Gamma^2 A}$	Keane and Horner		LUBRA	
		β	Ratio of Minima	β	Ratio of Minima
0	0	0.0994	1.0000	0.0948	1.0000
300	0.3432	0.0618	0.8420	0.0608	0.8449
600	0.6864	0.0481	0.7684	0.0463	0.7684
900	1.0296	0.0403	0.7190	0.0385	0.7196
1200	1.3729	0.0351	0.6822	0.0339	0.6831
1500	1.7161	0.0312	0.6529	0.0315	0.6543

TABLE 14

COMPARISON OF LUBRA WITH GYMEA VALUES OF THE TOTAL RESOLVED EFFECTIVE RESONANCE INTEGRAL OF U238 USING THE NARROW RESONANCE MODEL WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	T = 0 $^\circ$K		T = 300 $^\circ$K	
	LUBRA	GYMEA	LUBRA	GYMEA
1	5.753	5.753	5.973	5.978
5	6.713	6.713	7.010	7.018
10	7.747	7.747	8.139	8.150
50	13.372	13.372	14.512	14.537
100	18.056	18.057	20.096	20.123
200	24.845	24.846	28.587	28.588
500	38.342	38.343	46.616	46.395
1000	53.214	53.215	67.616	66.873
2000	73.251	73.253	96.356	94.706
5000	108.684	108.690	144.059	141.640
10,000	141.212	141.210	181.159	179.910

TABLE 15

COMPARISON OF LUBRA WITH GYMEA VALUES OF THE TOTAL RESOLVED EFFECTIVE RESONANCE INTEGRAL OF Th232 USING THE NARROW RESONANCE MODEL WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	T = 0°K		T = 300°K	
	LUBRA	GYMEA	LUBRA	GYMEA
1	2.383	2.383	2.703	2.712
5	2.710	2.710	3.141	3.154
10	3.070	3.070	3.652	3.660
50	5.094	5.094	6.775	6.799
100	6.809	6.809	9.726	9.710
200	9.300	9.300	14.238	14.085
500	14.203	14.203	23.069	22.518
1000	19.460	19.460	31.641	30.744
2000	26.202	26.202	40.806	39.833
5000	36.935	36.935	51.576	51.190
10,000	45.342	45.342	57.533	57.759

TABLE 16

COMPARISON OF LUBRA WITH GYMEA VALUES OF THE TOTAL RESOLVED EFFECTIVE RESONANCE INTEGRAL OF Pu240 USING THE NARROW RESONANCE MODEL WITH THE A.A.E.C. LIBRARY DATA

σ_M (barns)	T = 0°K		T = 300°K	
	LUBRA	GYMEA	LUBRA	GYMEA
10	95.19	95.21	95.43	95.69
100	223.13	223.13	225.02	225.54
500	479.44	479.47	487.71	488.51
1×10^3	673.02	673.05	687.28	688.32
5 "	1472.80	1472.80	1517.67	1522.20
1×10^4	2042.66	2042.70	2118.12	2125.40
2 "	2793.27	2793.30	2919.70	2929.00
5 "	4063.07	4063.10	4278.25	4293.70
1×10^5	5144.90	5145.0	5403.03	5435.1
2 "	6167.90	6167.9	6412.64	6467.5
5 "	7189.56	7189.6	7353.31	7412.0
1×10^6	7664.37	7664.4	7765.06	7803.1
1×10^7	8184.58	8184.6	8196.96	8208.2

TABLE 17

COMPARISON OF LUBRA WITH GYMEA VALUES FOR THE TOTAL RESOLVED DOPPLER COEFFICIENT AVERAGED OVER 300 DEG. KELVIN INTERVALS FOR U238, Th232 AND Pu240, USING THE MODIFIED-λ MODEL WITH THE A.A.E.C. LIBRARY DATA

ΔT	$-D_C \times 10^5$ for U238 ($\sigma_M = 10^6$ b)		$-D_C \times 10^5$ for Th232 ($\sigma_M = 10^3$ b)		$-D_C \times 10^5$ for Pu240 ($\sigma_M = 10^5$ b)	
	LUBRA	GYMEA	LUBRA	GYMEA	LUBRA	GYMEA
0 – 300	6.64	6.58	20.50	19.18	5.08	5.15
300 – 600	2.00	1.92	6.28	6.32	3.35	3.30
600 – 900	1.18	1.16	3.92	4.07	2.58	2.46
900 – 1200	0.83	0.82	2.84	3.02	2.11	1.97
1200 – 1500	0.62	0.63	2.22	2.40	1.78	1.65

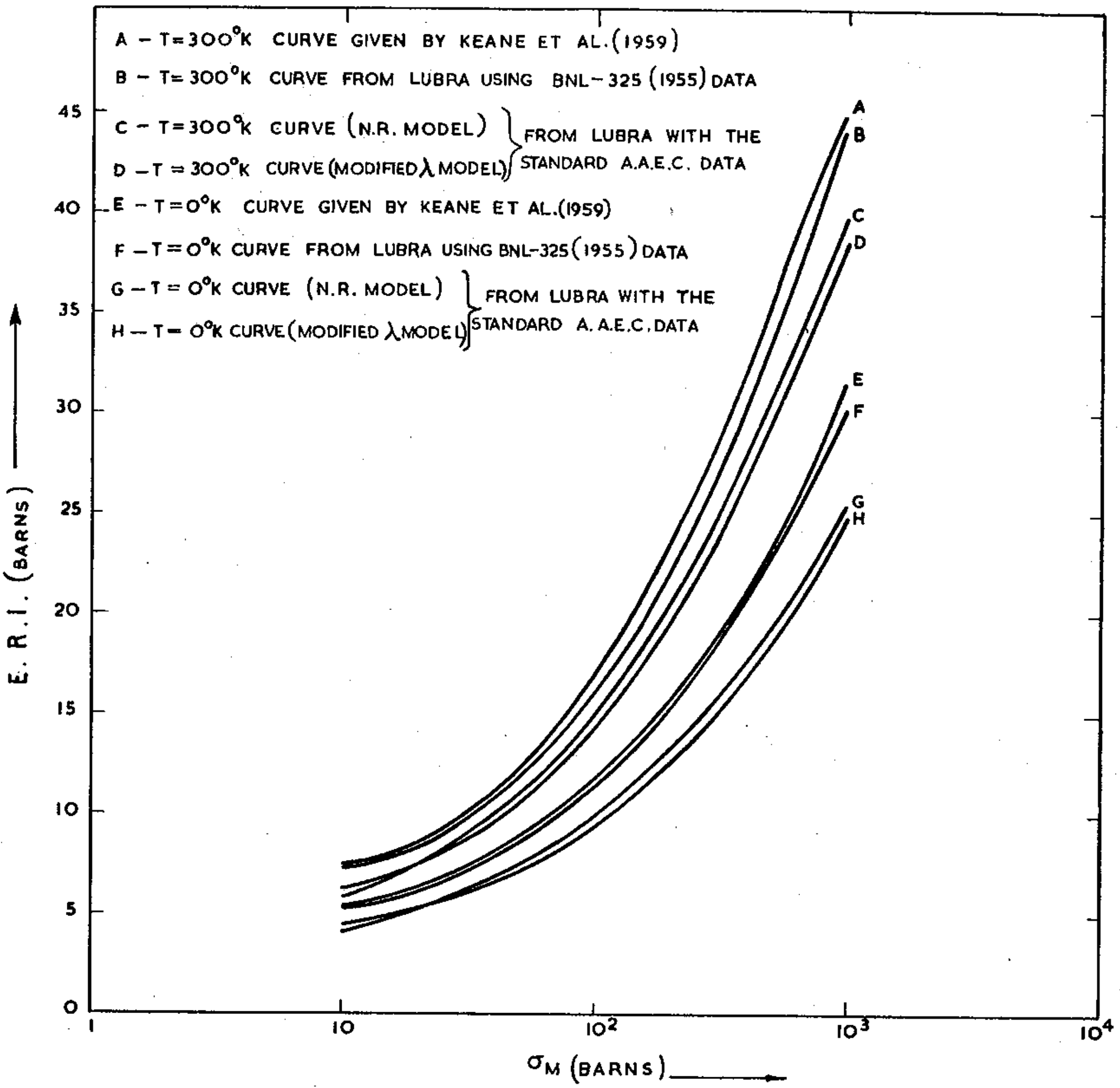

FIGURE 1. COMPARISON OF LUBRA EFFECTIVE RESONANCE INTEGRAL VALUES FOR Th232 AT T = 0° K AND 300°K WITH THOSE QUOTED BY KEANE ET AL.(1959)

P1048

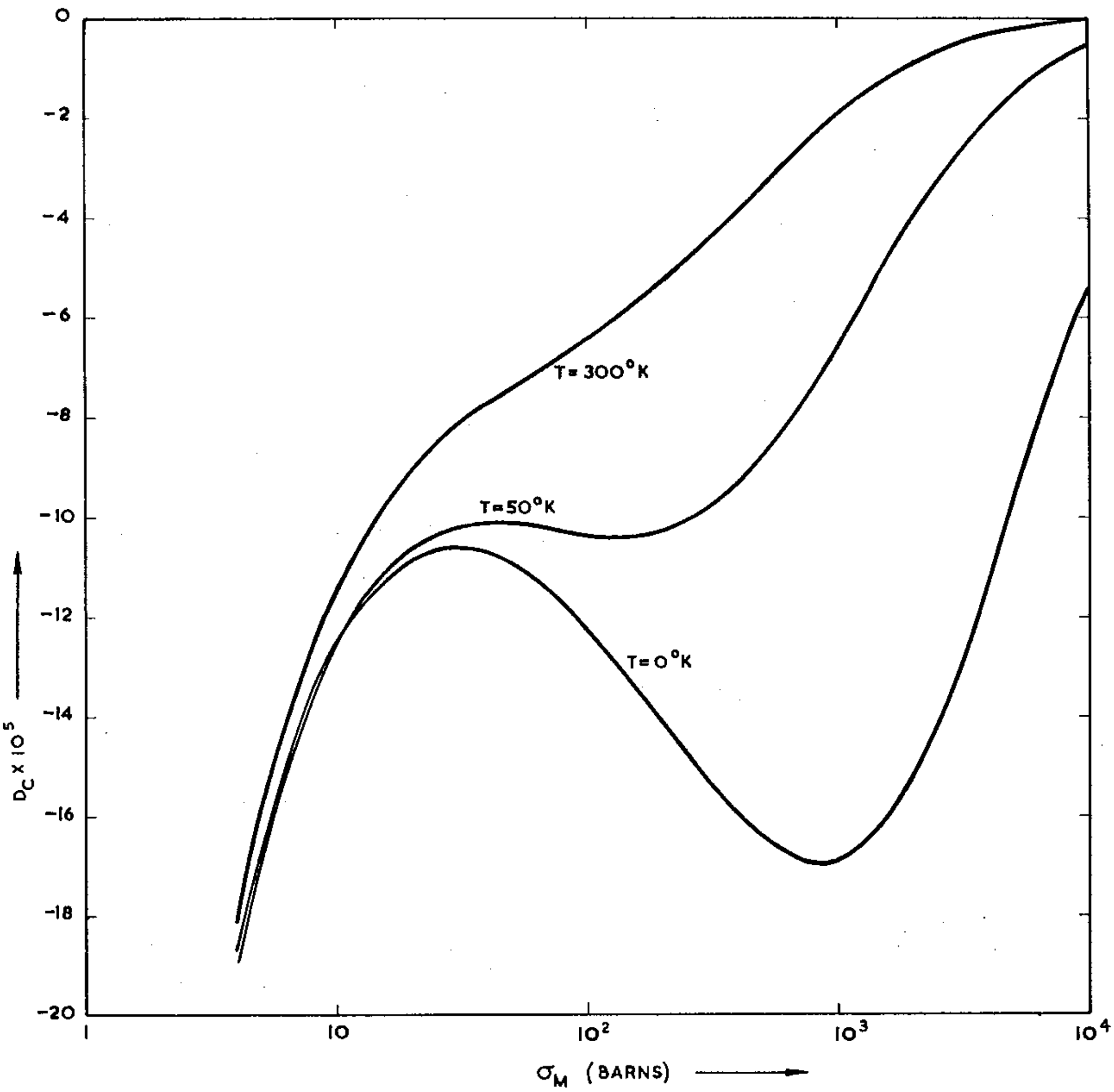

FIGURE 2. THE DOPPLER COEFFICIENT OF THE 22 eV RESONANCE OF Th232 AS A FUNCTION OF MODERATOR SCATTERING PER Th232 ATOM, USING THE NARROW RESONANCE MODEL AND A.A.E.C. LIBRARY DATA

P1046

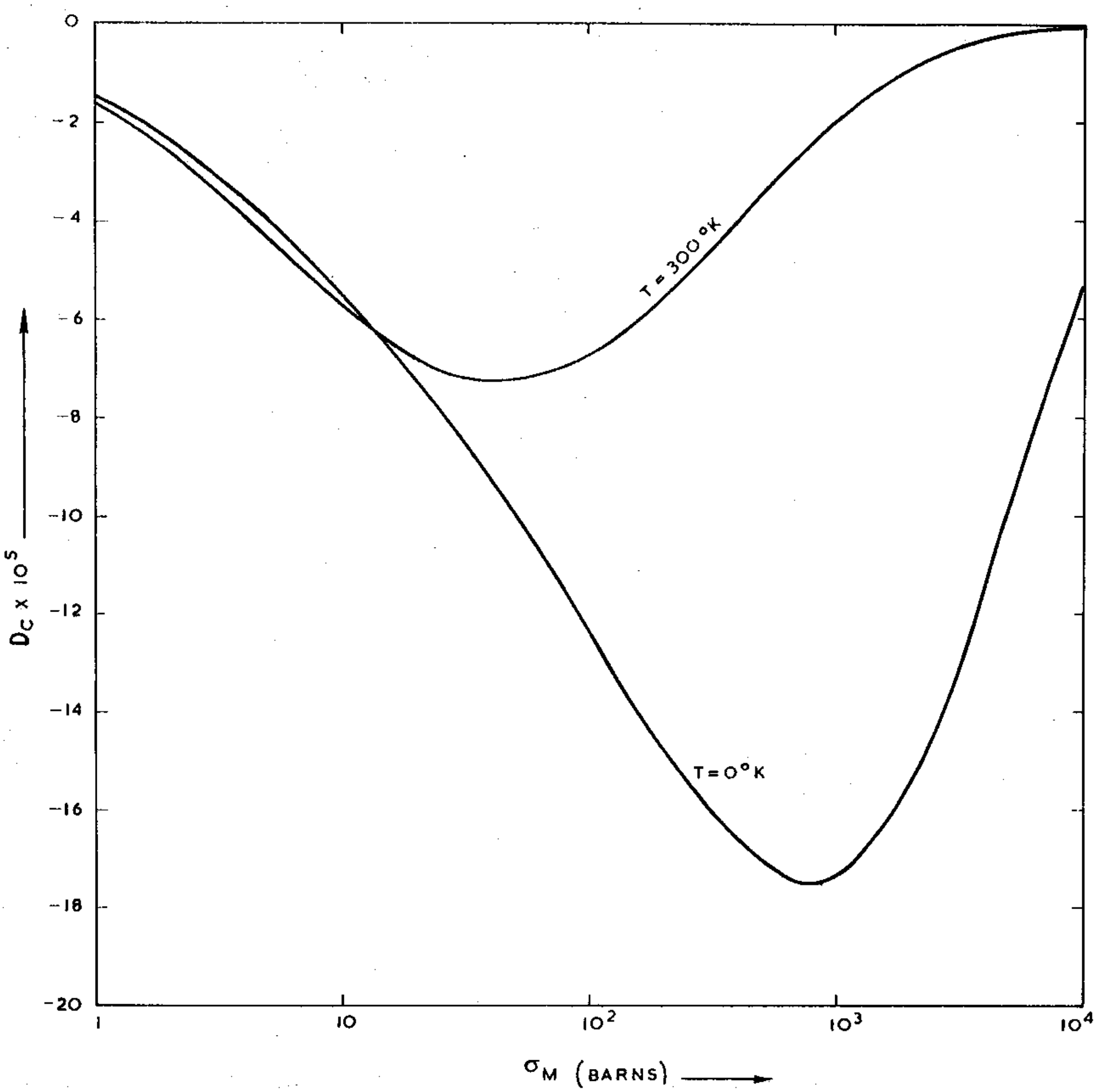

FIGURE 3. THE DOPPLER COEFFICIENT OF THE 22 eV RESONANCE OF Th232 AS A FUNCTION OF MODERATOR SCATTERING PER Th232 ATOM, USING THE MODIFIED-λ MODEL AND THE A.A.E.C. LIBRARY DATA

P1048

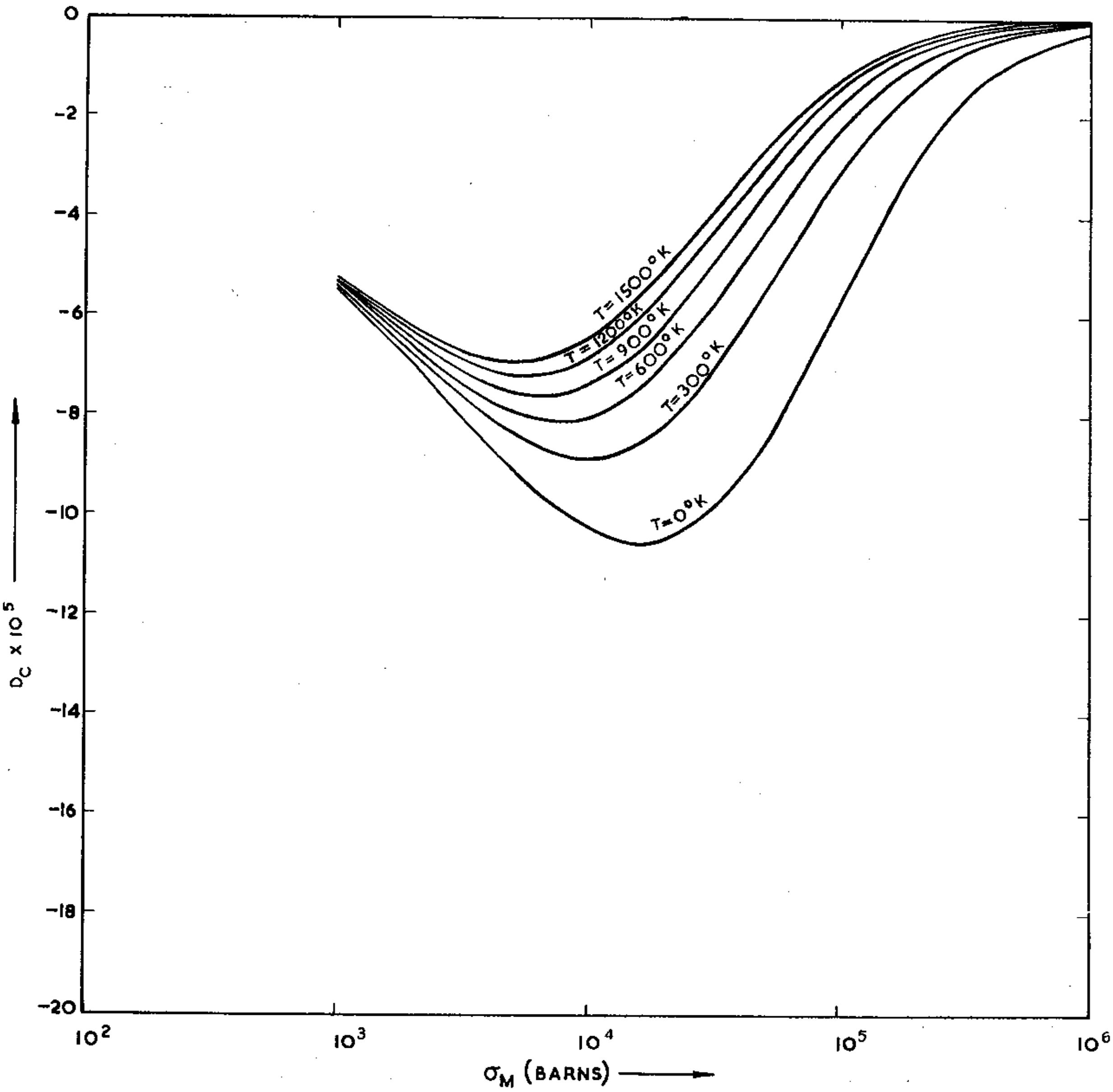

FIGURE 4. THE DOPPLER COEFFICIENT OF THE 1 eV RESONANCE OF Pu240 AS A FUNCTION OF MODERATOR SCATTERING PER Pu240 ATOM, USING THE NARROW RESONANCE MODEL AT T = 0(300)1500°K

P1048

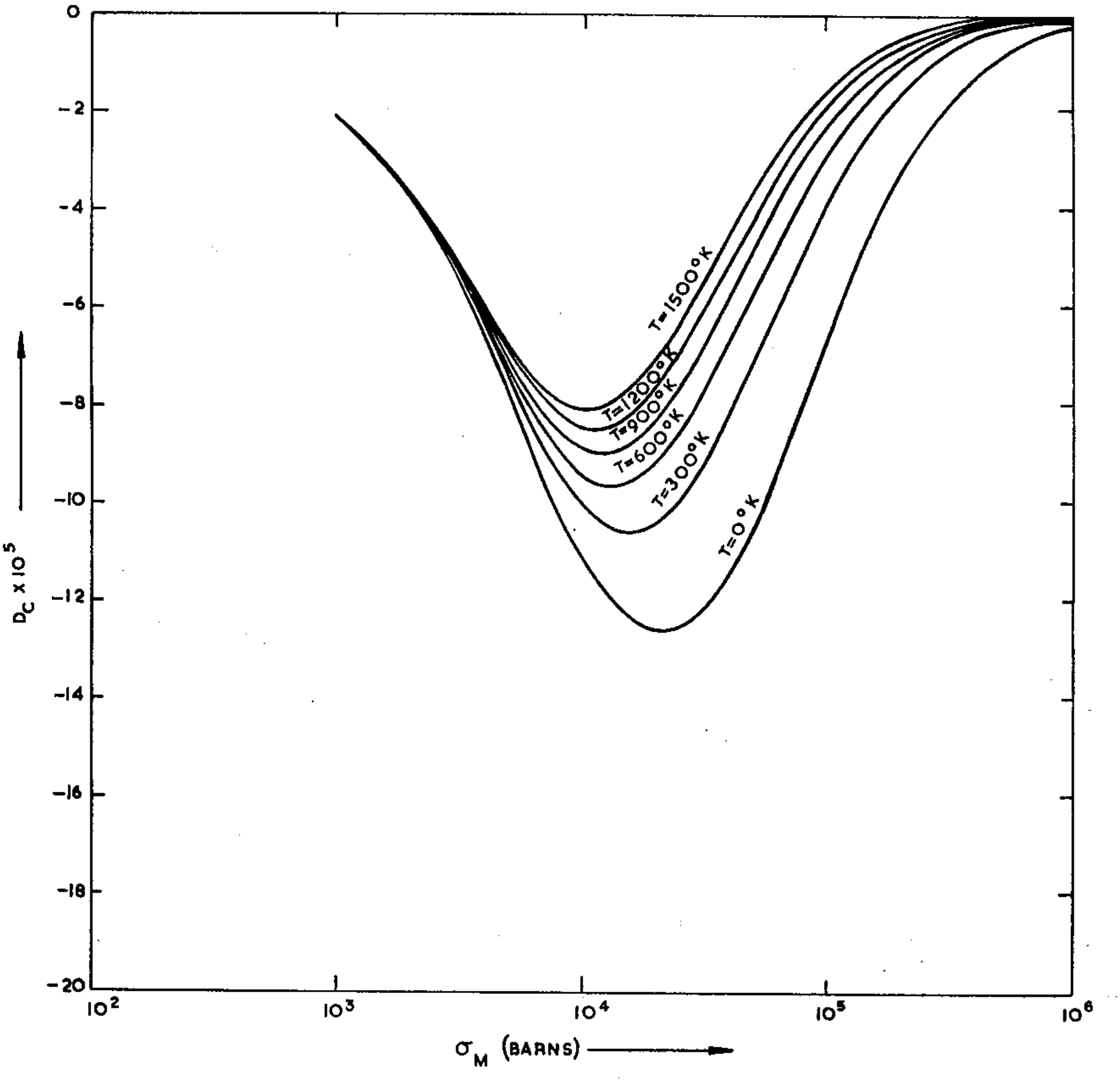

FIGURE 5. THE DOPPLER COEFFICIENT OF THE 1 eV RESONANCE OF Pu240 AS A FUNCTION OF MODERATOR SCATTERING PER Pu240 ATOM, USING THE MODIFIED-λ MODEL AT T = 0(300)1500°K

P1048

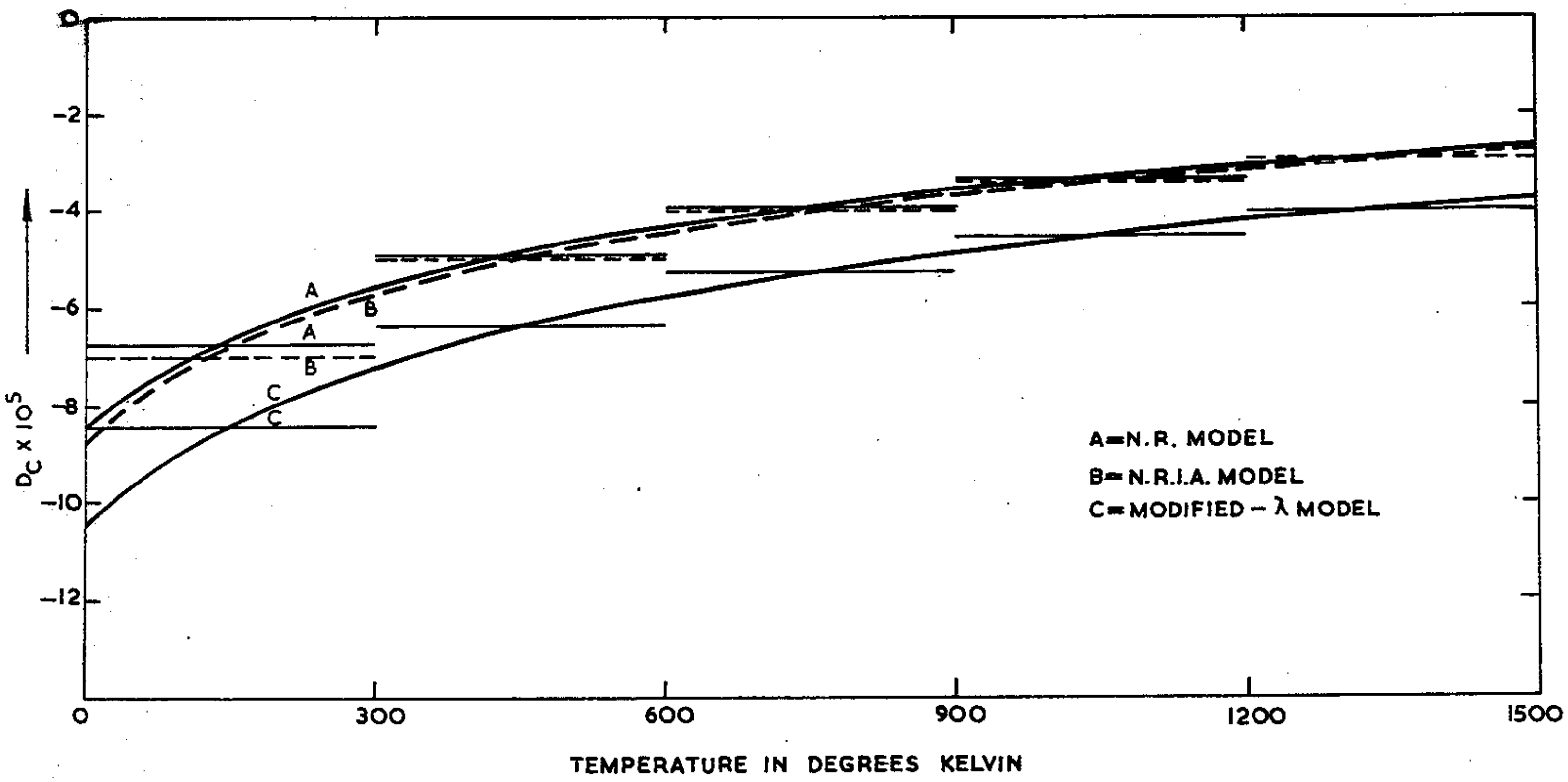

FIGURE 6. COMPARISON OF THE EXACT DOPPLER COEFFICIENT OF THE 1 eV RESONANCE OF Pu240 WITH AVERAGE VALUES OVER 300 DEGREE INTERVALS

P. 1048