Brief Report to JEF/EFF Meetings, Paris, 8-9 Dec. 1994
Subject: Evaluations with large negative File 3 corrections in the unresolved resonance region.

RESTORATION OF THE JEF EVALUATION OF ^{244}Cm IN THE UNRESOLVED RESONANCE REGION

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ABSTRACT. A KEDAK-4 evaluation for ^{244}Cm in the resolved and unresolved resonance region was adopted for JEF (and EFF) after translation to ENDF format with the conversion code KTOE. More recent checks revealed that the converted evaluation has abnormally high negative "background corrections" in File 3. Since in KEDAK there are no such corrections, and since the average resonance parameters had been correctly converted, there is no reason for any corrections, let alone large ones. Comparison with the original KEDAK version shows that the corrections had been, in fact, unnecessarily introduced. They were therefore removed completely. The constant old average parameters were slightly updated by (similar) energy-dependent parameters obtained by fitting the original KEDAK point data. It was verified that NJOY reproduces the correct point data from the evaluation thus restored. The complete corrected ^{244}Cm evaluation was sent to NEADB in June 1994.

1. Problems with Large "Corrections" in the Unresolved Resonance Region

When JEF-1 was assembled a number of KEDAK-formatted evaluations from KfK Karlsruhe and from RCN Petten were adopted, after reformatting with the conversion code KTOE at ENEA Bologna. More recently it was noticed that for the unresolved resonance region many of the files thus converted had abnormally high negative "background corrections" in File 3 (for capture cross sections), often of similar magnitude as the uncorrected capture cross sections that are calculated from the level-statistical parameters tabulated in File 2. This seemed strange since

- KEDAK has never employed "background corrections",
- the average resonance parameters had been correctly translated by ENEA about 1 MeV (in particular the strength functions to reduced neutron widths for the given mean level spacings and degrees of freedom),
- the formalism for the calculation of point cross sections from average resonance parameters is essentially the same in KEDAK and ENDF, viz. Hauser-Feshbach formulae with width fluctuation corrections derived in SLBW approximation (Dresner factors).

Inspection of the list of "bad" cases prepared by C. Nordborg, NEA Data Bank, showed that of all the entries only one, ^{244}Cm, was a KfK evaluation. Another one, ^{237}U from ENDF/B-V, hence not converted from KEDAK format, appears to be not "bad" at all: The only capture cross section listed with a large background correction lies right at the border between resolved and unresolved region, so it should not be regarded as the first point of the unresolved, but rather as the last point of the resolved resonance region – where, in fact, corrections can be relatively large in the (practically unimportant) valleys between resonances. All the other evaluations on the list were from RCN Petten. Because initially it was not clear whether the point data or the resonance parameters were to be blamed we restricted ourselves to ^{244}Cm which had been evaluated at KfK so that all the necessary information was at hand, in particular the level-statistical parameters and the corresponding point data for the total, capture, fission and inelastic scattering cross sections.

2. The KEDAK Evaluation of the Unresolved Resonance Region of ^{244}Cm

Statistical analysis with the STARA program (Fröhner 1983) had yielded a mean spacing for s-wave levels of

$$D_0 = 11.9 \pm 0.9\text{eV}$$

and an s-wave strength function of

$$S_0 = \left(1.07^{+0.31}_{-0.19}\right) \cdot 10^{-4} ,$$

whereas a spherical optical-model potential for actinides (Fischer 1980) had given

$$S_0 = (1.14 \pm 0.12) \cdot 10^{-4} .$$

This last strength function value was adopted for extrapolation of average cross sections into the low keV region. The average radiation width found from resolved s-wave resonances,

$$\Gamma_\gamma = 36.2\text{meV},$$

was used for the p- and d-wave levels, too. The other parameters used for the KEDAK point cross section calculation are listed in Table 8, where R_l^∞ are the distant-level parameters related to the effective channel radii, and E_f and$\hbar\omega$ are the height and the curvature parameter of a Hill-Wheeler fission barrier reproducing the (smoothed) fission cross section measured by Moore and Keyworth (1971). The cross sections calculated with these parameters are shown in Fig. 1.

Table 1 – Original KEDAK Parameters

ℓ	D_0 (eV)	S_ℓ (10^{-4})	R_ℓ^∞	$\overline{\Gamma}_{\gamma,\ell}$ (meV)	E_f (MeV)	$\hbar\omega$
0	11.9	1.14	−0.054	36.2	0.60	0.63
1		2.30	+0.150	36.2		
2		1.17	−0.045	36.2		

3. The "Background Corrections" in JEF

In the Comments in the JEF file for ^{244}Cm (Material 9637) it is stated that the translation from KEDAK to ENDF format was performed by ENEA Bologna with the conversion code KTOE. The main change involved is replacement of the strength functions in KEDAK by reduced neutron widths in ENDF. Likely errors in this step are (i) confusion between neutron widths and reduced neutron widths, (ii) mistakes with respect to the degrees of freedom for the neutron width distributions and width fluctuation corrections, (iii) erroneous units. It was found, however, that the converted parameters were correct.

Regarding File 3 "background corrections" the comments are not very helpful. They state only that corrections were calculated twice, in 1985 and 1989, but neither by whom and how nor why. Now File 3 "background corrections" are not allowed by the KEDAK format rules, as mentioned before, so they have never been employed in KEDAK files, nor should they be needed in the reformatted JEF versions.

4. The Restored File for ^{244}Cm and its Validation

A fit to the original KEDAK point cross sections with the Hauser-Feshbach code FITACS (Fröhner et al. 1982) gave essentially the old KEDAK parameters, modified somewhat by a weak energy dependence at higher energies. The parameters thus obtained were translated in ENDF format and put into a complete ^{244}Cm file from which *all FILE 3 "background corrections" were removed.* Total and partial cross sections for infinite dilution were calculated from this restored file

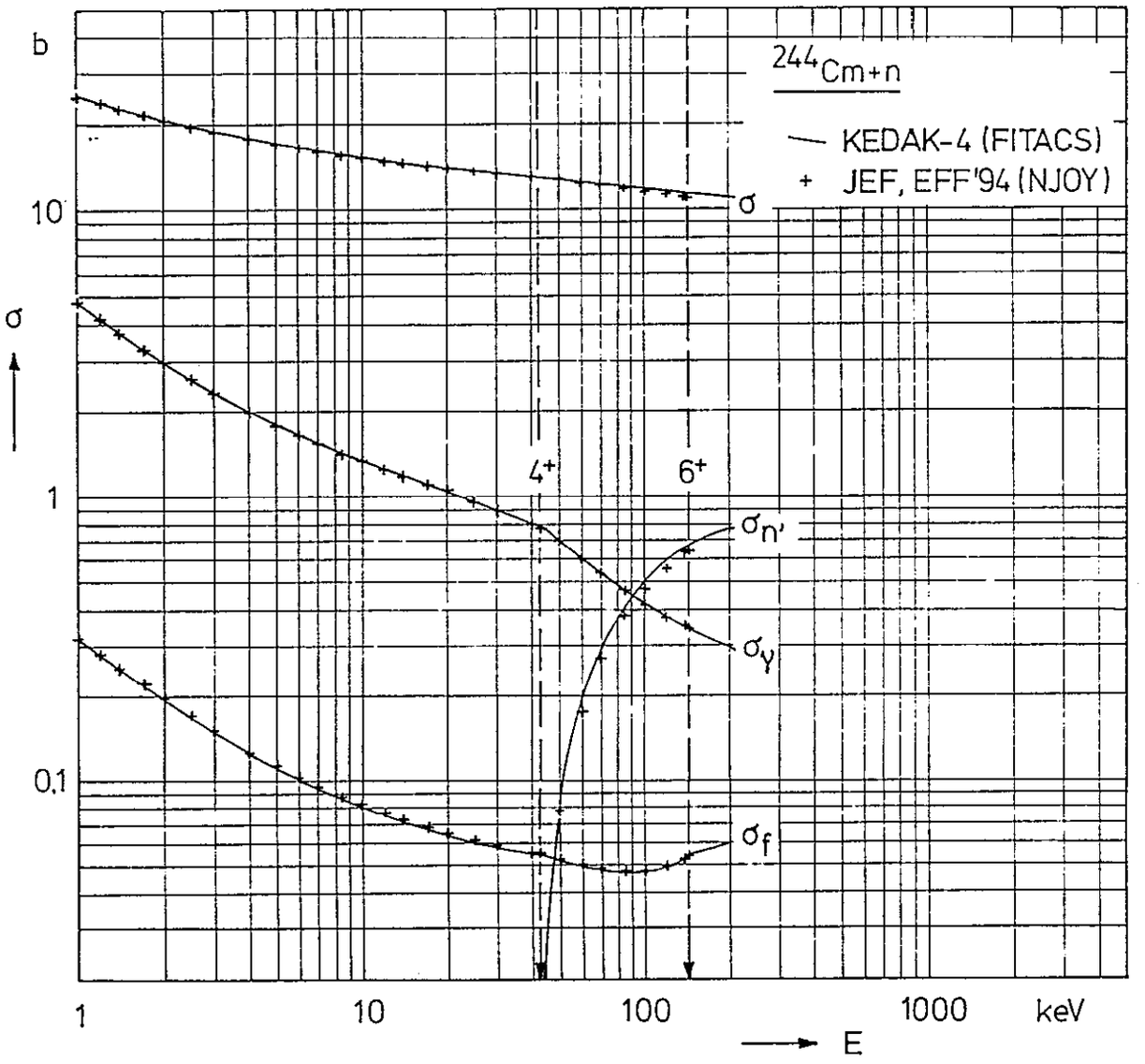

Fig. 1. –Original KEDAK evaluation for ^{244}Cm in the unresolved resonance region (curves) and point cross sections calculated from the restored JEF file by the NJOY module UNRESR (crosses). Thresholds for inelastic scattering are labeled by the spin-parity characteristics of the residual states.

with the modules UNRESR and GROUPR of NJOY-89.89. The resulting data points are shown in Fig. 1 together with the original KEDAK curves. The agreement is seen to be good, especially below the first (4^+) inelastic threshold. The small differences are due to a somewhat more sophisticated Hauser-Feshbach treatment in FITACS as compared to NJOY, for instance with respect to width-fluctuation corrections and number of inelastic channels. In any case the differences are well within the uncertainties of the original KEDAK evaluation which due to lack of transmission, capture and inelastic scattering data was largely an extrapolation from the resolved resonance region towards higher energies, based on level statistics obtained from resolved resonances, on the spherical optical-model potential for actinides established by Fischer (1980), and on the fission data of Moore and Keyworth (1971).

After the restored ^{244}Cm evaluation had been validated by cross section calculations with NJOY it was transmitted to the NEA Data Bank in June 1944, for inclusion in future updates of

JEF and EFF (instead of the "twice incorrectly corrected" present ^{244}Cm evaluation).

5. Other JEF/EFF Files with Large "Background Corrections"

The other JEF/EFF files with large negative "background corrections" were taken over from KEDAK-formatted RCN evaluations for fission products. The capture cross sections involved are model calculations by H. Gruppelaar and H.A.J. van der Kamp. After our experience with ^{244}Cm it is likely that the level-statistical parameters are correct, in the original KEDAK versions as well as in the ENDF versions. The decision whether this is true so that one can simply remove the File 3 "background corrections", or whether the cross sections calculated by NJOY are correct, can best be made by the authors of the evaluations.

ACKNOWLEDGMENTS

It is a pleasure to thank C. Nordborg, NEA Data Bank, for the list of JEF materials with large negative "background corrections" and other help, and Mrs. B. Krieg for validation of the restored ^{244}Cm file by means of cross section calculations with NJOY.

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