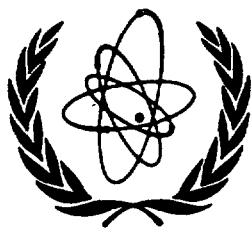




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**A STUDY INTO THE RELIABILITY OF COLLAPSING
SAND-II 640 MULTIGROUP DATA INTO VITAMIN-J 175
MULTIGROUP CROSS SECTIONS**

Prepared by

Harm WIENKE
IAEA Nuclear Data Section
Vienna, Austria

July 1995

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

VITAMIN-J 175 multigroup cross sections for the $^{55}\text{Mn}(n,\gamma)$, $^{58}\text{Fe}(n,\gamma)$ and $^{58}\text{Ni}(n,p)$ reactions, obtained by collapsing SAND-II 640 multigroup data, were compared with the VITAMIN-J 175 multigroup cross sections obtained by directly processing the pointwise cross sections for these reactions. The results showed significant discrepancies.

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Introduction

In the working group on production and interfacing of FENDL libraries to the ITER design the following discussion was recorded (Ref. 1): "The dosimetry data are based on IRDF-90 version 2 data provided in SAND-II multi-group form with 640 energy groups. The question of providing the data in continuous energy format was addressed. If the data are available in pointwise form from the original source (e.g. ^{197}Au from ENDF/B-VI), they will be processed from the point-wise data. Otherwise they will be processed from histogram representation". S. Ganesan suggested that it would be desirable to see if there is any effect of collapsing the 640 group IRDF data instead of going from the point data. The present report, which is an outcome of this suggestion, documents the results of an investigation into the reliability of collapsing SAND-II 640 multigroup data into VITAMIN-J 175 multigroup cross sections. The procedures and results of the calculations and the inter-comparisons, which have been made for some reaction cross sections, are presented.

Details of Calculations

Pointwise cross section data in ENDF-6 format for the $^{55}\text{Mn}(n,\gamma)$, $^{58}\text{Fe}(n,\gamma)$ reactions were derived from ENDF/B-VI with the NJOY code RECONR (Ref. 2). From these pointwise cross sections and from the ENDF/B-VI data for the $^{58}\text{Ni}(n,p)$ reaction multigroup cross sections were derived in 640 energy group SAND-II and in 175 energy group VITAMIN-J structure with the NJOY code GROUPR (Ref. 2) using a flat weighting spectrum (IWT=2 in GROUPR). Then the multigroup cross sections in SAND-II structure were collapsed into 175 energy group VITAMIN-J format using GROUPR again. Therefore these cross sections, which originally were in the GROUPR output (GENDF) format, were first converted into ENDF-6 histogram format (interpolation law 1), using a conversion code developed at the Nuclear Data Section, and then into ENDF-6 linear-linear interpolable format (interpolation law 2) using RECONR again, as GROUPR only accepts linear-linear interpolable cross section data as input. The thus obtained collapsed cross section data in 175 energy group VITAMIN-J structure and the VITAMIN-J multigroup cross sections obtained with GROUPR directly from the pointwise cross sections were also converted from GENDF format into ENDF-6 histogram format and plotted with the ENDF plotting and intercomparison code COMPLIT written by D.E. Cullen (Ref. 3). Figures 1-3 show the comparison plots for above mentioned reactions. The input parameters for NJOY are given in the appendix.

Results

For the $^{55}\text{Mn}(n,\gamma)$ reaction the VITAMIN-J multigroup cross sections resulting from collapsing the SAND-II data are in good agreement with those obtained by processing of the pointwise data directly with GROUPR in the energy regions from 0.01 meV up to 100 eV and from 100 keV up to 20 MeV. Between 100 eV and 0.1 MeV there is more than 50 percent discrepancy which is not acceptable (Fig. 1). A similar picture as in Fig. 1 is shown in Fig. 2 for the $^{63}\text{Cu}(n,\gamma)$ reaction: agreement in the energy regions from 0.01 meV to 400 eV and from 100 keV to 20 MeV. Between 400 eV and 100 keV the multigroup cross sections differ even up to a factor ten. For the $^{58}\text{Ni}(n,p)$ threshold reaction (Fig. 3) the discrepancy between both VITAMIN-J multigroup cross sections is smaller - up to 7 percent for some groups between 0.5 and 2.4 MeV, which, however, is also still not acceptable.

Concluding Remarks

In general collapsing a fine group structure into a coarse one is only allowed when the coarse group energy boundaries are a subset of the fine group ones (Ref. 4). However, the effect of using non coincident boundaries will be small when the number of fine groups per energy interval is much larger than that of the coarse groups or when the original pointwise cross sections do not vary much with energy. This is clearly demonstrated by the fair agreement between the collapsed VITAMIN-J cross sections and those obtained directly from the pointwise data for both (n,γ) reactions in the energy region .01 meV up to 100 eV, which is covered by about 270 SAND-II groups versus only 24 VITAMIN-J groups, and at energies above the resolved resonance region (about 100 keV), where the cross section is a smooth function of the neutron energy (see figures 1 and 2). In the energy region 100 eV up to 100 keV, however, where the numbers of both groups are much closer to each other and where the original pointwise data fluctuate rather much with neutron energy - i.e. in the resolved resonance region, the effect of using non coincident energy boundaries is more serious, as is shown in the above mentioned figures. The fact that for the $^{58}\text{Ni}(n,p)$ reaction (Fig. 3) the effect of using non coincident boundaries in collapsing the SAND-II multigroups into VITAMIN-J multigroups is not very large may probably be attributed to the rather smooth pointwise cross section.

All calculations with GROUPR also have been performed using a VITAMIN-E neutron weighting spectrum. The results turned out to be essentially the same as those obtained using a flat neutron weighting spectrum.

From the above discussed results it may be concluded that generation of VITAMIN-J 175 multigroup cross sections by collapsing SAND-II 640 multigroup data is not recommendable.

References

1. S. Ganesan, (ed.), "Improved Evaluations and Integral Data Testing for FENDL" Summary report of the IAEA Advisory Group Meeting organized by the International Atomic Energy Agency in co-operation with the Max-Planck Institut für Plasmaphysik, Garching, Germany, 12-16 September 1994, report INDC(NDS)-312, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria.
2. R.E. MacFarlane, "The NJOY Nuclear Data Processing System, Version 91", Los Alamos National Laboratory report LA-12740-M, to be published.
3. D.E. Cullen, "The 1994 ENDF Pre-processing Codes", report IAEA-NDS-39, Rev. 8, January 1994, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria.
4. D.E. Cullen, "Nuclear Cross Section Processing", Handbook of Nuclear Reactor Calculation, Vol. 1, CRC Press, inc., Boca Raton, Florida (in Press).
5. C.L. Dunford, "ENDF Utility Codes Release 6.9", report IAEA-NDS-29, Rev. 6.9, Nov. 1993, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria.

Appendix: NJOY Input Parameters

The input parameters for NJOY/RECONR and GROUPR as used for the $^{55}\text{Mn}(n,\gamma)$ reaction, with tape 20 as the ENDF/B-VI cross section input data file, tape 22 the RECONR pointwise cross section output data file and tape 25 the VITAMIN-J multigroup GENDF output file, were as follows:

```
0
6
*RECONR*
20 22
* Mn-55 FROM ENDF/B-VI */
2255 2/
.001 0. 7 .001 1.0E-15
* Mn-55 FROM ENDF/B-VI*/
* PROCESSED WITH NJOY91.* /
0/
*GROUPR*
20 22 0 25
2525 17 0 2 0 1 1 0 / matb ign igg iwt lord ntemp nsigz iprint
*Mn-55 (n,g) GROUPR, VITJ 175 multigroup data*/
0.
1.E10
3 102/
0/
*STOP*
```

The GROUPR input parameters for generating SAND-II multigroup data were the same except for the neutron group structure option "ign", which was set on 15. The multigroup GENDF output files (tape 25) were converted into the ENDF-6 format with the NDS code CONV_ENDF and the ENDF utility code STANEF (Ref. 5). As the SAND-II multigroup cross section data files (in ENDF-6 format), before being processed into VITAMIN-J group structure by GROUPR, had to pass RECONR, which reads in resonance parameters, these were headed by a file 1, with LRP set to zero, and a dummy file 2 containing only the scattering radius AP.

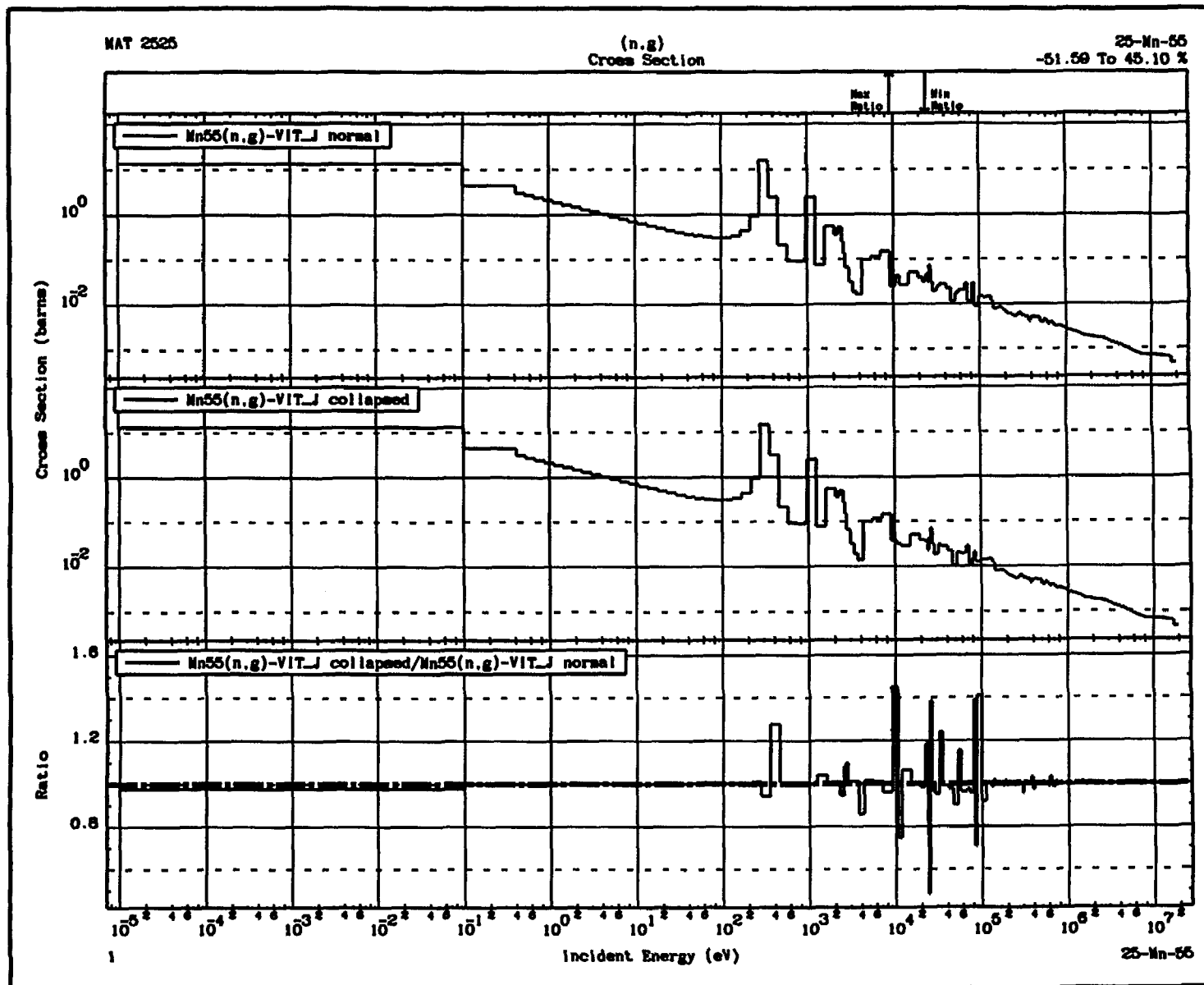


Fig. 1 VITAMIN-J multigroup cross sections for the $^{55}\text{Mn}(n,\gamma)$ reaction derived with RECONR/GROUPR from ENDF/B-VI normally versus the ones obtained by collapsing the SAND-II 640 multigroup cross section data.

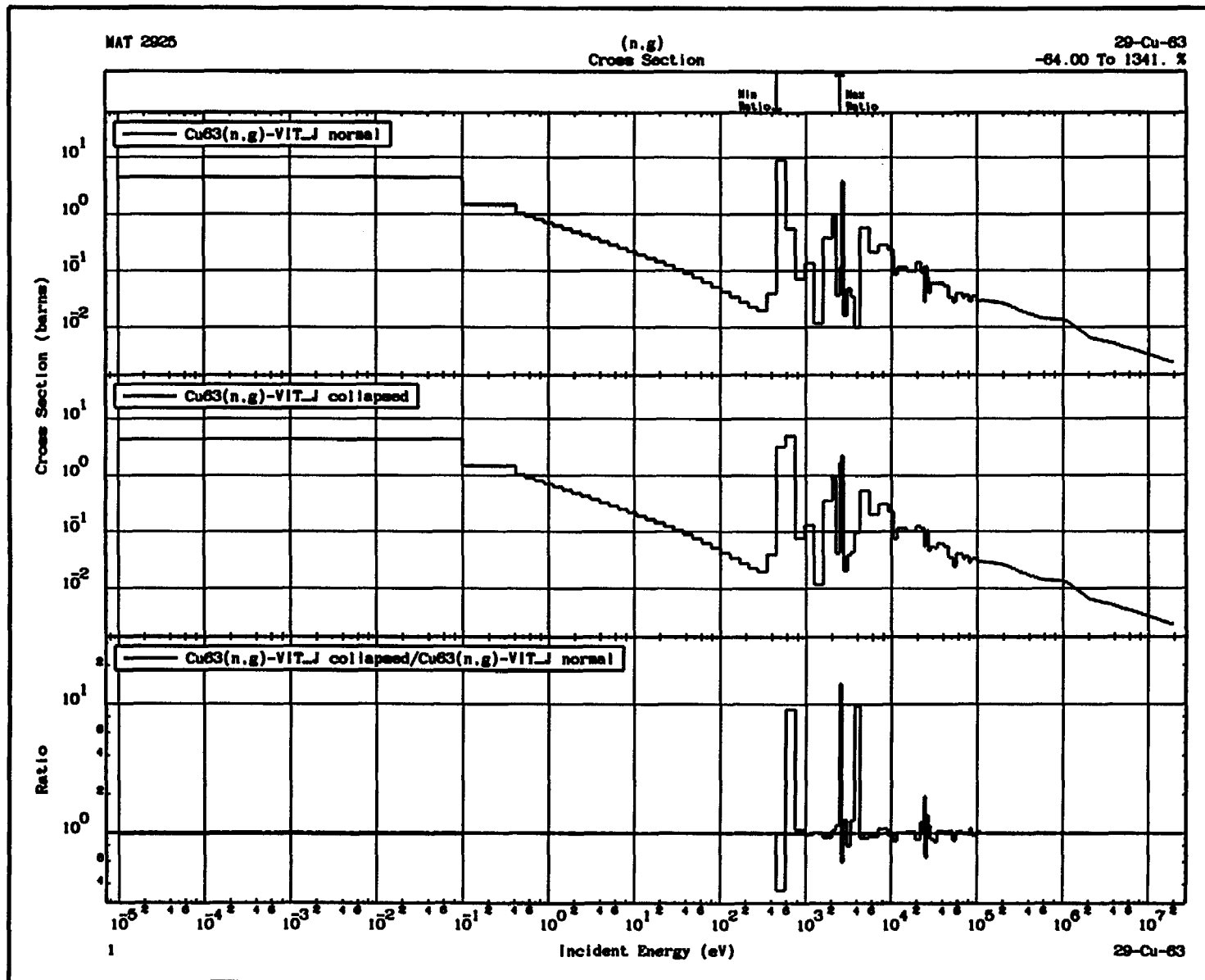


Fig. 2 VITAMIN-J multigroup cross sections for the $^{63}\text{Cu}(n,\gamma)$ reaction derived with RECONR/GROUPR from ENDF/B-VI normally versus the ones obtained by collapsing the SAND-II 640 multigroup cross section data.

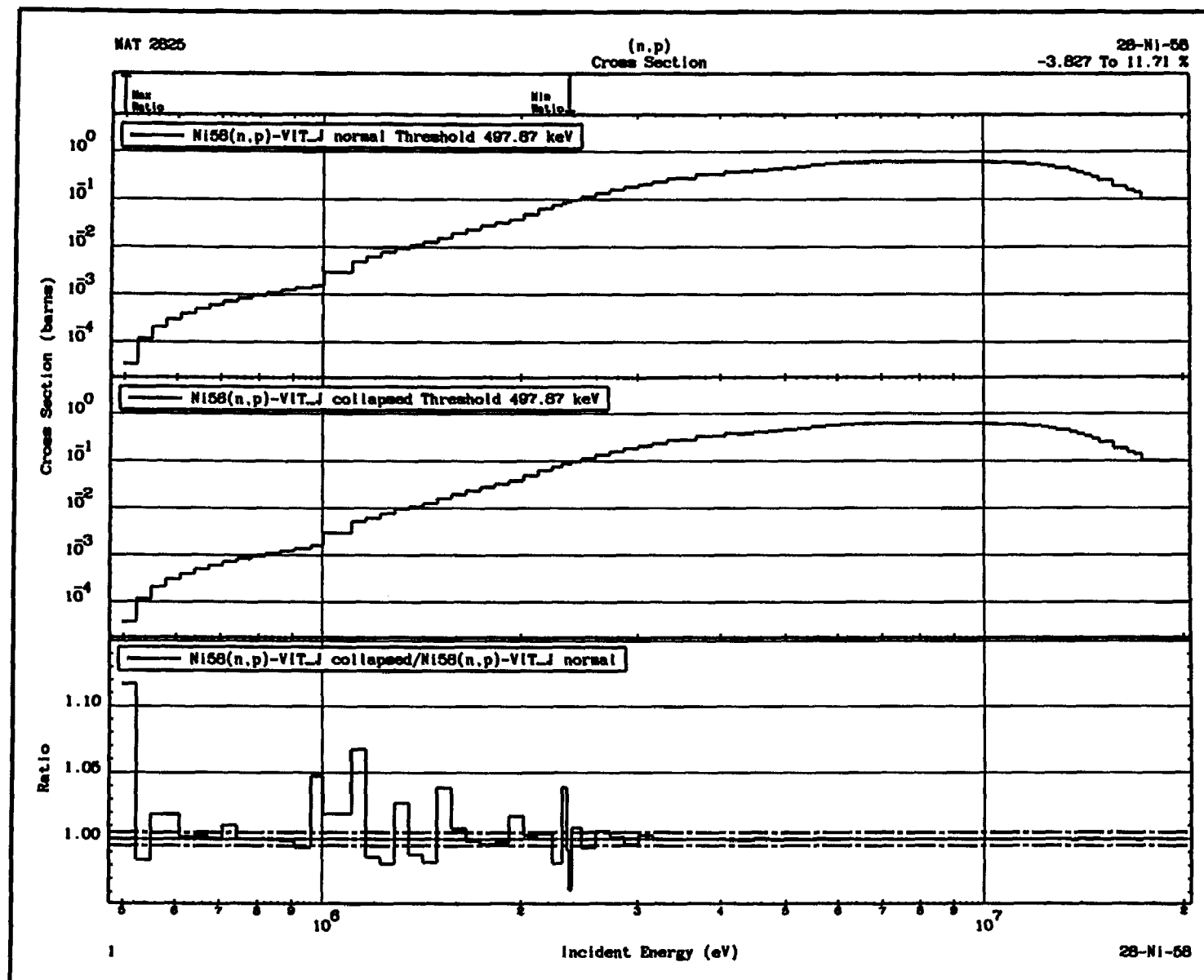


Fig. 3 VITAMIN-J multigroup cross sections for the $^{58}\text{Ni}(n,p)$ reaction derived with RECONR/GROUPR from ENDF/B-VI normally versus the ones obtained by collapsing the SAND-II 640 multigroup cross section data.