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Compilation of the *"Atlas of Gamma-rays from the Inelastic Scattering of Reactor Fast Neutrons"* (1978DE41) by A. M. Demidov, L. I. Govor, Yu. K. Cherepantsev, M. R. Ahmed, S. Al-Najjar, M. A. Al-Amili, N. Al-Assafi, and N. Rammo

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Abstract

A Structured Query Language (SQL) relational database has been developed based on the original $(n, n'\gamma)$ work carried out by A. M. Demidov *et al.*, at the Nuclear Research Institute in Baghdad, Iraq [*"Atlas of Gamma-Ray Spectra from the Inelastic Scattering of Reactor Fast Neutrons"*, Nuclear Research Institute, Baghdad, Iraq (Moscow, Atomizdat 1978)] for 105 independent measurements comprising 76 elemental samples of natural composition and 29 isotopically-enriched samples. The information from this ATLAS includes: γ-ray energies and intensities; nuclide and level data corresponding to where the γ-ray originated from; target (sample) experimental-measurement data. Taken together, this information allows for the extraction of the flux-weighted $(n, n'\gamma)$ cross sections for a given transition relative to a defined value. Currently, we are using the fast-neutron flux-weighted partial γ-ray cross section from ENDF/B-VII.1 for the production of the 847-keV $2^+_1 \rightarrow 0^+_{\mathrm{gs}}$ transition in ^{56}Fe, $\sigma_\gamma = 468$ mb. This value also takes into account contributions to the 847-keV transition following β^- decay of ^{56}Mn formed in the ^{56}Fe(n, p) reaction. However, this value can easily be adjusted to accommodate the user preference. The $(n, n'\gamma)$ data has been compiled into a series of ASCII comma separated value tables and a suite of Python scripts and C modules are provided to build the database. Upon building, the database can then be interacted with directly via the SQLite engine or accessed via the Jupyter Notebook Python-browser interface. Several examples exploiting these utilities are also provided with the complete software package.

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Inelastic neutron scattering is the primary energy-loss mechanism for fast neutrons in heavy ($A > 12$) nuclei. As such, a good knowledge of it is required for virtually all branches of applied nuclear science ranging from shielding calculations to the design of advanced nuclear-energy systems to international security and counter proliferation. The need for improved neutron-scattering data was explicitly stated in the recent white paper [1] from the Nuclear Data Needs and Capabilities for Applications Workshop. In addition to its utility for nuclear applications, $(n, n'\gamma)$ provides unique insight into off-yrast nuclear structure due to the non-selective nature of the reaction (which can include a significant compound component) and the wide range of angular momentum states accessible to fast neutrons.

Angle-differential (n, n') data is notoriously difficult to measure due to the difficulties involved in measuring the neutron energy and the lack of intense neutron beams. An alternate approach to determining $(n, n'\gamma)$ cross sections involves measuring the prompt γ rays emitted from the excited states populated via inelastic scattering, e.g., (n, n'). While these measurements lack the angle-differential information needed to improve neutron transport, they can provide an important integral constraint to the nuclear-reaction evaluation process and can be used to improve modeling for nondestructive assay of materials using active neutron interrogation.

The *"Atlas of Gamma-rays from the Inelastic Scattering of Reactor Fast Neutrons"* published by A. M. Demidov *et al.*, [2] is one of the most comprehensive compilations of data on $(n, n'\gamma)$ in existence containing over 7000 γ rays from 76 natural and 29 isotopically-enriched targets. The data in the Atlas comes from a single Li-drifted Ge γ-ray detector located on a filtered "fast" neutron beam line at the IRT-5000 reactor formerly located at the Al-Tuwaitha research facility outside of Baghdad, Iraq. All of the data in the "Baghdad Atlas" was taken using the same Ge γ-ray detector and the same experimental configuration. Detailed information regarding the target areal density was provided, allowing all the transition intensities to be normalized to the partial γ-ray cross section for inelastic scattering to the first excited state in ^{56}Fe at 847 keV. While the details of the neutron spectrum are not completely known, the experimental setup was designed to minimize the presence of low-energy thermal neutrons. Their success is evident in that there are only 30 transitions in the Atlas firmly assigned to (n, γ) reactions. The authors reference earlier work [3] indicating the energy dependence of the fast neutron spectrum is of the form $\exp(-\beta E_n)$ where $\beta = 0.6 - 0.7$ and E_n is the neutron energy (MeV).

In order to determine the best value for the flux-weighted $^{56}\text{Fe}(n, n'\gamma_{847})$ cross section we convolved the spectrum for the IRT reactor shown in Figure 5 of the Atlas [2] with the value for the $^{56}\text{Fe}(n, n'\gamma_{847})$ cross section taken from ENDF/B-VII.1 [4]:

$$\langle\sigma\rangle = \frac{\int_0^{E_n=20} \phi(E_n)\sigma_\gamma(2_1^+)dE}{\int_0^{E_n=20} \phi(E_n)dE}, \tag{1}$$

where $\phi(E_n)$ is the flux from the Atlas and $\sigma_\gamma(2_1^+)$ is the partial γ-ray cross section for the 847-keV $2_1^+ \rightarrow 0_{\text{gs}}^+$ transition.

There is an additional contribution to the 847 keV transition which can be attributed

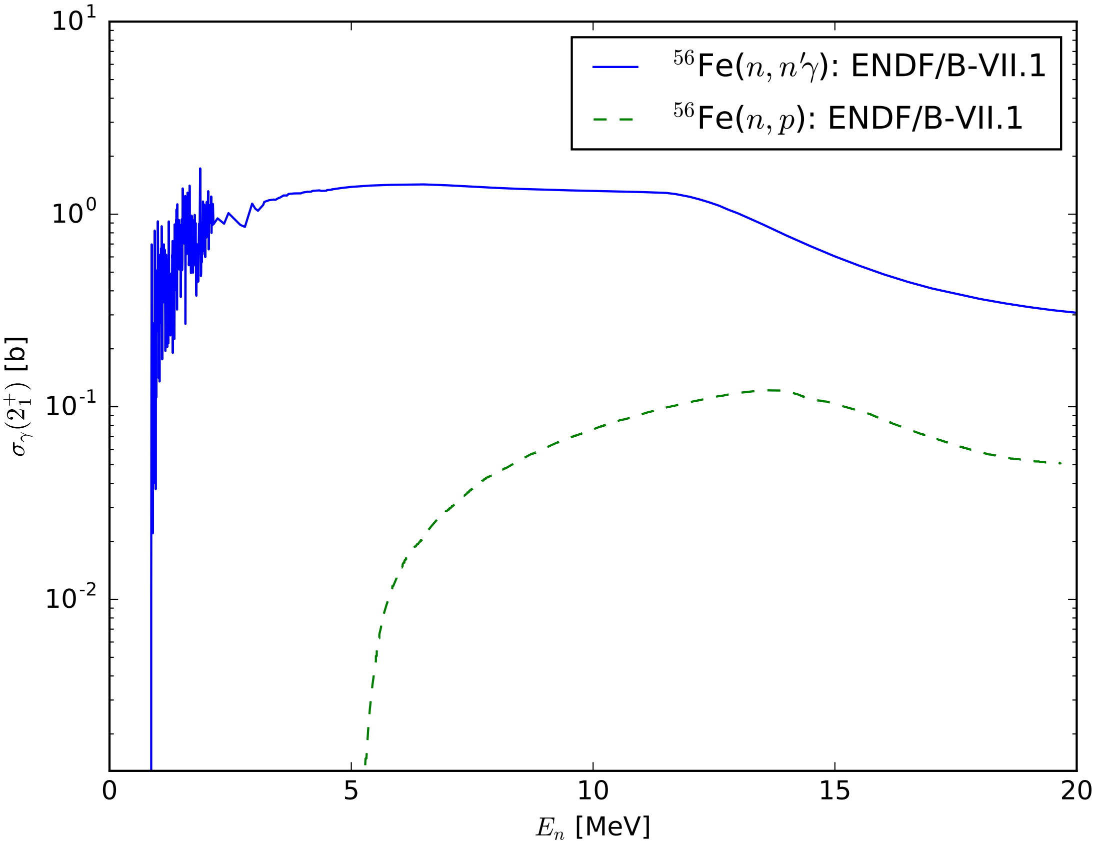

Figure 1: Cross-section data [4] for the ^{56}Fe$(n, n'\gamma_{847})$ and ^{56}Fe(n, p) reactions.

to the β^- decay of ^{56}Mn formed in the ^{56}Fe(n, p) reaction, which produces the ^{56}Fe 847-keV γ-ray transition with a 98.85% branching ratio [5]. This contribution can be calculated using the same approach given in Eq. (1) because the experiment was performed over a long period of time compared to the lifetime of ^{56}Mn ($t_{1/2} \approx 2.6$ h [5]), allowing it to come into secular equilibrium. This contribution has been estimated, using the ENDF/B-VII.1 value for the (n, p) cross section as 2.34% of the $(n, n'\gamma_{847})$ value. Figure 1 shows the energy-differential cross sections for the ^{56}Fe$(n, n'\gamma_{847})$ and the ^{56}Fe$(n, p)^{56}$Mn cross sections from ENDF/B-VII.1 [4] used. Taking this into account together with the natural-abundance of ^{56}Fe (91.754% [6]) we obtain a spectrum-averaged, decay-corrected value of 468 mb for $\langle\sigma\rangle$.

The data in the Atlas is valuable for many applications ranging from nuclear nonproliferation, active neutron-interrogation studies and benchmarking nuclear-reaction models in the fast-fission neutron range. However, its use is limited by the fact that the data was only available in printed form. The nuclear data group at the Lawrence Berkeley National Laboratory and UC Berkeley have compiled the data into a set of comma separated value ASCII tables and an SQLite (structured query language) database for dissemination to increase the accessibility for the international community. The complete package may be downloaded and contains the following:

- Scripts to compile the data into a SQLite database for both Python 2 and Python 3. The Makefile provided will test for the appropriate version and run with the necessary settings.
- A C-code to produce the extension-functions library allowing for mathematical functions such as sine, cosine, logarithm, square root etc. to be invoked with SQL methods. These are not standard functions with the SQLite3 engine. The Makefile will establish the correct OS-kernel name and compile the library accordingly.
- The complete set of CSV data files compiled for 76 different nuclei in the range $3 \leq Z \leq 92$. This includes data sets from 76 natural samples and 29 isotopically-enriched samples (105 data sets in total).
- An example Jupyter Notebook illustrating methods for interacting with and visualizing the data.
- Several SQL scripts showing database-interaction examples. The OS-dependent library will be defined in SQL methods where appropriate during the make run phase of the installation.
- A PDF of the ATLAS [2] provided for reference.
- An HTML manual describing the software installation procedure and data-access methods. An overview of the ATLAS data is also provided in this documentation.

This first release of the Atlas database is designed to serve the needs of the application community. The energy levels, γ-ray energies and intensities are those stated in the Atlas itself and have not been reconciled to match those in the current version of the Evaluated Nuclear Structure Data File (ENSDF), although state-of-the-art structure information has been used to identify γ-ray doublets (reported as unresolved doublets for now). Our intention is to issue periodic revisions where the γ-ray and level-scheme information for specific nuclei has been updated to match modern values in ENSDF, and we encourage users of the atlas to assist in this process by sending updated csv data to the Berkeley group <LABernstein@lbl.gov> for more general dissemination to the user community.

In addition to its immediate use to the application community, the Atlas can serve as a valuable resource to both the nuclear structure and reactions evaluations communities. Since (n, n') at fast-reactor neutron energies proceeds via both direct and compound processes it provides a nonselective insight into the properties of off-yrast levels over a far wider range of spins than thermal and epithermal neutron capture. This property of (n, n') has made it an attractive area of research to many research groups in the international nuclear science community. This is exemplified by the plethora of papers on ^{56}Fe$(n, n'\gamma)$ by groups from Russia [7], Los Alamos [8, 9], GELINA [10], and Dresden [11].

Lastly, we hope that this SQLite database will provide a useful tool for the reactions evaluation community by providing easy access to angle-integrated data to aid in the benchmarking process needed for the validation of Evaluated Nuclear Data File libraries.

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