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Activity Report of the ENEA Nuclear Data Project in 2009

Prepared by

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March 2010

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Activity Report of the ENEA Nuclear Data Project in 2009

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Abstract

Descriptions are given of the nuclear data activities undertaken during 2009 at the Bologna Research Centre of the Italian National Agency for New Technologies, Energy and the Environment (ENEA).

March 2010

TABLE OF CONTENTS

Nuclear Structure Theory

Algebraic models of chiral doublets in odd-odd nuclei

Doublets of $\Delta I = 1$ bands almost degenerate in energy have been observed in odd-odd nuclei in the $A \sim 105$, $A \sim 130$ and $A \sim 190$ mass regions. They have been interpreted as chiral doublets in a geometrical model where a triaxial even-even core is coupled to a high-j particle-like proton and a high-j hole-like neutron (or vice versa) and the angular momenta of the core, the odd proton and the odd neutron form a mutually orthogonal right-handed or left-handed triplet in the intrinsic reference frame. This static picture of chirality is not present in the interacting boson-fermion-fermion model (IBFFM) of odd-odd nuclei [C.1], where the even-even cores in the above mentioned mass regions are not statically triaxial, but rather soft with respect to γ vibrations, and the yrast and yrare bands forming the doublets in odd-odd nuclei have a different dynamical structure. Similar conclusions can be drawn in the recently developed ortho-symplectic extension of the interacting vector boson model [A.1, C.2].

Fig. 1 compares the experimental yrast and yrare bands of ^{134}Pr built on the $\pi h_{11/2} \, x \, \nu h_{11/2}$ two-quasiparticle configuration with calculations performed with the interacting boson-fermion-fermion model (IBFFM) and the orthosymplectic exension of the interacting vector boson model (Th): the latter results reproduce better the experimental levels up to high spin.

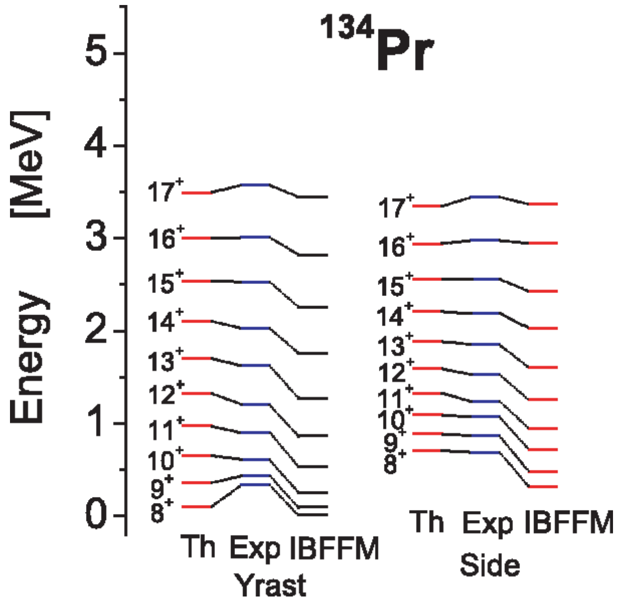

Fig.1. Calculated and experimental bands of ^{134}Pr built on the $\pi h_{11/2} \, x \, \nu h_{11/2}$ configuration.

The characteristics of the levels are better illustrated by intra-band transitions. Figs. 2 and 3 compare experimental and theoretical *B(E2)* and *B(M1)* transitions, respectively, in the yrast band. Here again, the best agreement with experimental data is obtained in the orthosymplectic extension of the interacting vector boson model.

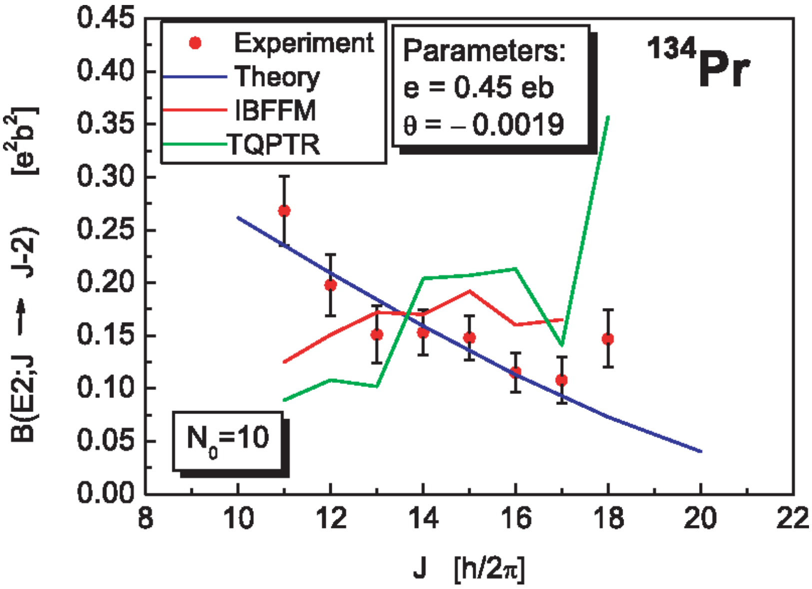

Fig. 2. Experimental and calculated B(E2) transitions between levels in the yrast band of ^{134}Pr vs. spin. Theory: orthosymplectic extension of the interacting vector boson model; IBFFM: interacting boson-fermion-fermion model; TQPTR: two-quasiparticle-plus-triaxial-rotor model.

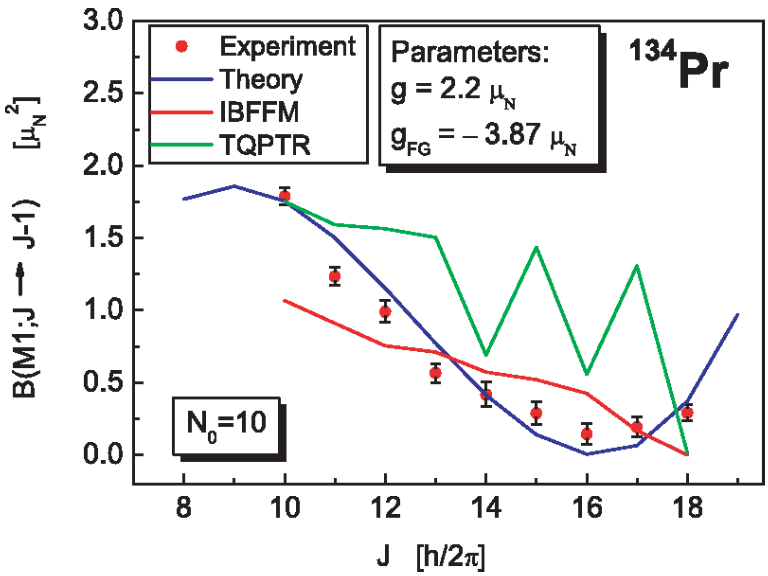

Fig. 3. Experimental and calculated B(M1) transitions between levels in the yrast band of ^{134}Pr vs. spin. Theory: orthosymplectic extension of the interacting vector boson model; IBFFM: interacting boson-fermion-fermion model; TQPTR: two-quasiparticle-plus-triaxial-rotor model.

Level density of ^{234}U

Within the framework of the analysis of the n_TOF (n,f) cross section of ^{233}U (see the following section on nuclear reaction theory and experiments) use has been made of a micro-canonical model of nuclear level densities already applied to transitional samarium isotopes in order to evaluate the average spacings of *s*- and *p*-wave resonances in the ^{233}U(n,f) reaction [C.3].

The total level density of the compound nucleus ^{234}U at excitation energies of the order of the neutron binding energy, $B_n \sim 6.845$ MeV, is obtained by convolution of a collective and a

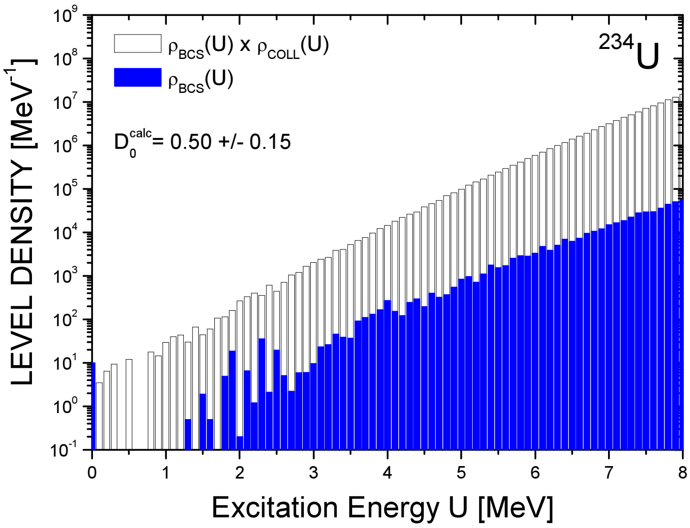

Fig. 4. Total level density of ^{234}U vs. excitation energy. Blue histogram: non-collective level density. Open histogram: total level density.

non-collective state density. The collective contribution is computed by means of the interacting boson model and reproduces the main bands of the discrete spectrum below the first two-quasiparticle excitation (ground-state, β, γ and octupole bands). The non-collective contribution is obtained by a Monte Carlo algorithm combining recursive state densities of non-interacting fermions with neutron-neutron and proton-proton pairing interactions in the standard Bardeen-Cooper-Schrieffer (BCS) approximation. Fig. 4 shows the non-collective density, $\rho_{BCS}(U)$, and the total density, including the collective enhancement factor, versus excitation energy, U.

The *s*-wave resonance spacing, D_0 , is computed in an interval of 600 eV above B_n from the densities of levels with spin-parity $J^\pi = 2^+$ and 3^+, while the *p*-wave resonance spacing, D_1, receives contributions from the densities of levels with $J^\pi = 1^-$,..., 4^- in the same energy interval, corresponding to an experimental resolved resonance region. The calculated values are $D_0 = (0.50 \pm 0.15)$ eV, which compares well with the values in the literature, and $D_1 = (0.25 \pm 0.10)$ eV.

Nuclear Reaction Theory and Experiments

Measurements of neutron cross sections at the n_TOF facility, CERN

The main experimental result published by the n_TOF Collaboration in 2009 is the (n,f) cross section of ^{233}U in the neutron energy range from 30 meV to about 1 MeV [A.2, C.4]. The cross section has been determined relative to a reference sample of ^{235}U(n,f) measured simultaneously with the same detector, a dedicated fission ionization chamber.

The n_TOF results in the unresolved resonance region from a few tens of keV to 1 MeV are shown in Fig. 5 together with results from previous measurements: up to approximately 200 keV, the n_TOF data are mostly consistent with previous measurements; above this energy, the previous data do not follow a common trend. In the same figure, the evaluated cross section from the ENDF/B-VII.0 library appears to be about 10% lower than the n_TOF cross section.

For clarity's sake, Fig. 6 shows the ratios of the n_TOF cross section and the evaluated cross sections from the ENDF/B-VII.0 and JEFF-3.1 libraries in the energy range from thermal to 1

MeV. The experimental data are significantly higher than the evaluated data in the interval from 10 eV to 0.1 MeV, where better agreement exists with the Oak Ridge measurements, by Guber *et al.*

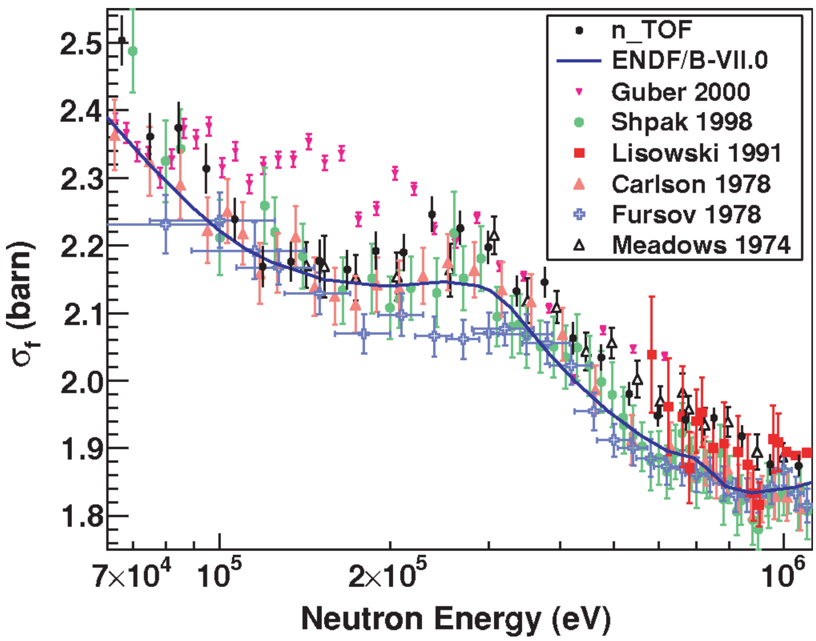

Fig. 5. Experimental ^{233}U(n,f) cross section in the neutron energy range from 70 keV to 1 MeV.

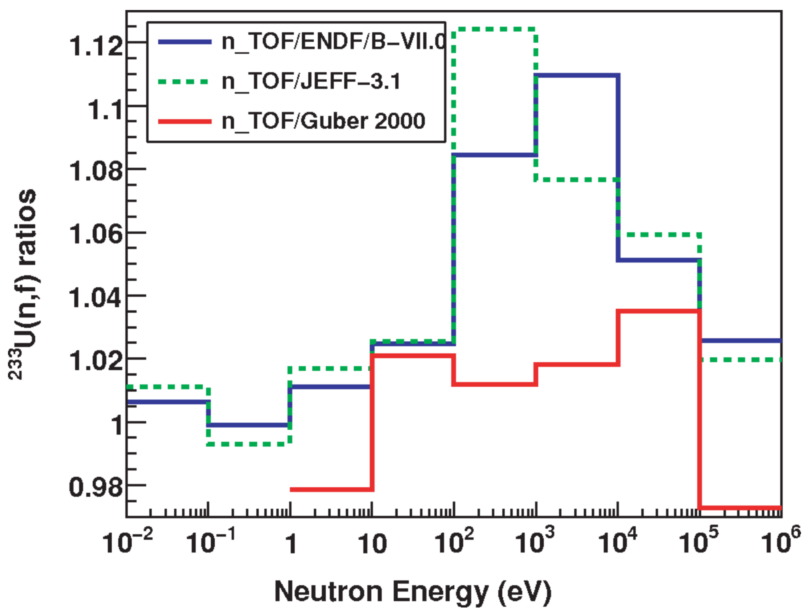

Fig. 6. Ratios of the n_TOF cross section and previous measured (Guber 2000) or evaluated cross sections.

The analysis of the resolved resonance region (E_n < 600 eV) is in progress and has motivated the level density calculations of the compound nucleus ^{234}U described in the preceding section.

As for neutron capture measurements, a detailed description of the total absorption calorimeter (TAC) has been published, together with preliminary results obtained with it [A.3]. The TAC is a segmented 4π detector array made of 40 BaF_2 crystals for (n,γ) cross section measurements and is especially designed for measuring cross sections of low-mass and/or radioactive isotopes because of its high efficiency and background rejection capabilities. Differently from the C_6D_6 liquid scintillation counters used in previous capture measurements, the TAC is designed to absorb the γ-ray cascade following neutron capture completely, with efficiency as independent as possible of the decay scheme of the compound nucleus.

The test measurements have been performed with three different samples: a stable element (^{197}Au), a radioactive element (^{237}Np) and natural carbon, which served as a pure scatterer. The tests have confirmed that the TAC is a powerful tool for measuring neutron capture cross sections of small and/or radioactive samples with high capture-to-background ratios and high detection efficiency.

Nuclear Data Processing and Validation

Nuclear data processing and validation activities, dedicated to fine and broad-group cross section libraries for nuclear fission applications, were performed in co-operation with a specialist presently working at the Kurchatov Institute of Moscow and formerly at the Institute of Physics and Power Engineering of Obninsk (Russian Federation).

In particular, the fine-group coupled neutron and photon MATJEFF31.BOLIB library in the ORNL VITAMIN-B6 neutron and photon energy group structures (199 neutron groups + 42 photon groups) was updated. In fact, this pseudo-problem-independent library in MATXS format, based on the JEFF-3.1 evaluated data library, was processed a short time before the release of the JEFF-3.1.1 data. The package of this processed library for nuclear fission applications, in agreement with the specific request of the OECD/NEA Data Bank, was equipped with an additional set of JEFF-3.1.1 processed data files, obtained for consistency with the same NJOY-99.160 (GROUPR module revised in ENEA-Bologna) system, previously used for the others JEFF-3.1 data. In particular, it was decided to reprocess only the 12 nuclides already inserted in the list of processed files for MATJEFF31.BOLIB whose evaluations were updated or corrected in the JEFF-3.1.1 library: ^{16}O, ^{35}Cl, ^{46}Ca, ^{52}Cr, ^{56}Fe, ^{91}Zr, ^{96}Zr, ^{95}Mo, ^{154}Eu, ^{233}U, ^{237}Np and ^{239}Pu. Further data validation work for the JEFF-3.1.1 processed files was performed on about 30 plutonium criticality benchmark experiments, comparing in particular the k-effective results obtained in one-dimensional deterministic transport calculations using the JEFF-3.1 Pu-239 cross sections of MATJEFF31.BOLIB and the revised JEFF-3.1.1 Pu-239 cross sections. These results were included in the user manual [R.1] of MATJEFF31.BOLIB which was prepared in parallel. The updated library and the dedicated user manual were transferred to OECD/NEA Data Bank, which presently distributes freely the package of the library with the denomination NEA-1847 ZZ MATJEFF31.BOLIB.

A new fine-group pseudo-problem-independent coupled neutron and photon library in AMPX format, named VITJEFF311.BOLIB and based on the JEFF-3.1.1 nuclear data, was generated with the NJOY-99.259 and the SCAMPI (ENEA-Bologna Revision 2007) nuclear data processing systems in the VITAMIN-B6 neutron and photon energy group structures previously indicated. VITJEFF311.BOLIB, in particular, was validated on the same set of about 30 plutonium benchmark experiments used to test the JEFF-3.1 and JEFF-3.1.1 processed files of the MATJEFF31.BOLIB library previously cited.

VITJEFF311.BOLIB was then collapsed in the neutron and photon energy group structures

(47 neutron groups + 20 photon groups) of BUGLE-96, an ORNL working library specifically dedicated to LWR shielding and pressure vessel dosimetry applications, through the SCAMPI (ENEA-Bologna Revision 2007) nuclear data processing system and proper PWR and BWR neutron and photon weighting spectra. In particular, the BUGJEFF311.BOLIB working library of self-shielded cross sections in FIDO-ANISN format was generated, specifically dedicated to LWR shielding and pressure vessel dosimetry applications. The package of the BUGJEFF311.BOLIB library was equipped with the whole set of 71 dosimetry cross sections, obtained from the point-wise cross section files of the International Reactor Dosimetry File IRDF-2002. The cross sections were, in particular, processed [R.2] in the 47 neutron group structure of the BUGLE-96 library through the GROUPIE program of the PREPRO 2007 package, using a pre-calculated neutron spectrum, specifically obtained with a one-dimensional transport calculation using JEFF-3.1.1 properly self-shielded cross sections, at 1/4 of the thickness of a specific PWR pressure vessel.

An equivalent set of data was prepared to equip the library package of BUGENDF70.BOLIB, a similar BUGLE-type library in progress, based on the ENDF/B-VII.0 evaluated nuclear data library. In conclusion, the response functions were calculated for all the following weighting spectrum conditions:

- flat weighting neutron spectrum;
- 1/4 T (T = PWR pressure vessel thickness) pressure vessel neutron weighting spectrum obtained from transport calculations using fine-group processed cross sections from the JEFF-3.1.1 evaluated nuclear data library;
- 1/4 T pressure vessel neutron weighting spectrum obtained from transport calculations using fine-group processed cross sections from the ENDF/B-VII.0 evaluated nuclear data library.

Finally, a contribution [C.5] was presented at the IAEA/OECD/NEA Technical Meeting on "Specific Applications of Research Reactors: Provision of Nuclear Data", (Vienna, Austria, October 12-16, 2009) in order to contribute to the promotion of the use of the broad-group working cross section libraries and three-dimensional deterministic transport codes in fission reactor shielding applications. In particular, it was proposed that IAEA and OECD/NEA should cooperate in creating an international forum of experts in nuclear and reactor physics in order to suggest to the national data processing working groups the most suitable group structures to be used in shielding applications for the various types of fission reactors (LWR, SFR, LFR, HTR, etc.) of current interest.

Computer Code Development

BOT3P Version 5.4 (BOT3P-5.4) was prepared in 2009. It will be transferred to the OECD/NEA Data Bank in the near future.

BOT3P is a set of standard FORTRAN 77 language codes developed at the ENEA Nuclear Data Group as from August 1997 and is designed to run on Linux/UNIX platforms. BOT3P Version 1.0 was originally conceived as a set of standard FORTRAN 77 language programs in order to give the users of the DORT and TORT deterministic transport codes some useful diagnostic tools to prepare and check their input data files for both Cartesian and cylindrical geometries, including mesh grid generation modules, graphical display and utility programs for post-processing applications. Later versions extended the possibility to produce the geometrical, material distribution and fixed neutron source data to other deterministic transport codes such as TWODANT and THREEDANT (both included in the DANTSYS

American package of deterministic codes), PARTISN (the updated parallel version of DANTSYS), the sensitivity code SUSD3D (distributed by OECD/NEA Data Bank) and, potentially, to any transport code through BOT3P binary output files that can be very easily interfaced. See, for example, the Westinghouse Electric Co. parallel radiation transport code RAPTOR-M3G (RApid Parallel Transport Of Radiation--Multiple 3D Geometries) and the Russian two and three-dimensional discrete ordinates neutron, photon and charged particle transport codes KASKAD-S-2.5 and KATRIN-2.0. BOT3P allows users to model X-Y, X-Z, Y-Z, R-Θ and R-Z geometries in two dimensions and X-Y-Z and R-Θ-Z geometries in three dimensions.

BOT3P was systematically and successfully used in 2009 in ENEA to generate the R-Θ-Z geometrical models in the IRIS (International Reactor Innovative and Secure) shielding analysis of the vessel by deterministic methods.

The IRIS application involved some important additions to BOT3P that are now included in Version 5.4, such as enhanced performances as post-processor of the TORT code.
A more efficient module to produce tetrahedron mesh grids starting from voxelized geometries, which might be particularly useful in medical applications, was studied and will be implemented in BOT3P in the future.

BOT3P has got large world-wide diffusion and is currently used by important companies such as, for example, Westinghouse Electric Co. and Ansaldo Nucleare.

Publications 2009

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