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Development of a Database for Prompt γ-ray Neutron Activation Analysis

Summary Report of the First Research Coordination Meeting
IAEA Headquarters, Vienna, Austria
2 to 4 November 1999

Prepared by
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Gaithersburg, Maryland, USA

February 2000

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Abstract

This report summarizes the presentations, recommendations and conclusions of the First Research Co-ordination Meeting on Development of a Database for Prompt γ-ray Neutron Activation Analysis. Neutron-capture Prompt γ-ray Activation Analysis (PGAA) is a non-destructive radioanalytical method, capable of rapid or in-situ simultaneous multielement analysis of many elements of the Periodic Table, from hydrogen to uranium, in the same sample. Inaccuracy and incompleteness of the data available for use in PGAA are a significant handicap in the qualitative and quantitative analysis of complicated capture-gamma spectra.

The goal of this CRP is to replace the twenty-year-old data from a single laboratory with something fundamentally new: an evaluated database which includes a combination of evaluated nuclear physics data, physical theory, and recent measurements. The resulting database will be comparable in quality with that for radioactive decay. In addition, more accurate values of neutron capture cross-sections and γ-ray intensities that result from this database will improve the accuracy of radiation shielding calculations.

February 2000

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1. SUMMARY OF THE MEETING

The First Research Co-ordination Meeting (RCM) on Development of a Database for Prompt γ-ray Neutron Activation Analysis was held at the IAEA Headquarters in Vienna, Austria, from 2 to 4 November 1999.

Neutron-capture Prompt γ-ray Activation Analysis (PGAA) is a non-destructive radio-analytical method, capable of rapid or in-situ simultaneous multielement analysis of many elements of the Periodic Table, from hydrogen to uranium, in the same sample. Inaccuracy and incompleteness of the data available for use in PGAA are a significant handicap in the qualitative and quantitative analysis of complicated capture-gamma spectra. The goal of this CRP is to replace the previously used tabulation of twenty-year-old data from a single laboratory with something fundamentally new: an evaluated database which includes a combination of evaluated nuclear physics data, physical theory, and recent measurements made within the scope of CRP. The resulting database will be comparable in quality with that for radioactive decay. Accurate PGAA measurements will be facilitated. In addition, more accurate values of neutron capture cross sections and γ-ray intensities that result from this database will improve the accuracy of radiation shielding calculations.

The purpose of the meeting was to work out a detailed working plan of the Coordinated Research Project (CRP), including tasks and responsibilities of participating laboratories, and agree on future coordination procedures. Richard B. Firestone of Lawrence Berkeley National Laboratory, USA, was elected as the chairman and Richard M. Lindstrom of National Institute of Standards and Technology (NIST), USA as rapporteur of the meeting. The detailed approved Agenda is attached (see Appendix 1). Other participating laboratories were represented by H.D. Choi (Seoul, Korea), A. Goswami (Mumbai, India), G.L. Molnár (Budapest, Hungary), V.H. Tan (Hanoi, Vietnam) and C. Zhou (Beijing, China). For the complete list of participants including affiliations see Appendix 2.

D.W. Muir, Head of the Nuclear Data Section (NDS), IAEA, gave a brief explanation of the general framework procedures under which the CRPs of the Agency develop (see Appendix 3) . R. Paviotti-Corcuera, Scientific Secretary of the CRP, summarised the overall objective of the CRP and the purpose of the meeting (see Appendix 4). The detailed Information Sheet of the CRP is given in Appendix 5. For the extended abstracts of the technical papers presented by participants see Appendix 6.

2. BACKGROUND

The International Nuclear Data Committee, at its 1997 meeting in Vienna, strongly recommended that the Nuclear Data Section support the update of the database and new measurements of data needed in neutron-induced Prompt γ-ray Activation Analysis (PGAA) (See Minutes of the 21st meeting of the International Nuclear Data Committee, February 1997, Report INDC/P(97)-20).

The increasing importance of PGAA and its broad range of applicability are evident and have been emphasised at many meetings related to this topic, e.g., the Technical Consultant Meeting held at Vienna, 4-7 May 1993 (Use of neutron beams for low and medium flux research reactors: radiography and materials characterisation, Report IAEA-TECDOC-837, 1993).

The Advisory Group Meeting on the Co-ordination of the Nuclear Structure and Decay Data Evaluators Network held at Budapest, 14-18 October 1996 (Report INDC(NDS)-363) stated that there is a need for a complete and consistent library of cold and thermal neutron-capture γ-ray and corresponding cross section data and recommended the organization of a CRP on the subject.

Inaccuracy and incompleteness of the data available for use in PGAA are a significant handicap in the qualitative and quantitative analysis of complicated gamma spectra. The basic source of information on thermal neutron capture γ-ray data for nuclides is the Evaluated Nuclear Structure and Decay Data File (ENSDF). Online access to the data is possible from the National Nuclear Data Center at Brookhaven, the IAEA Nuclear Data Section and other Centers. This file contains both isotope-specific measurements made for elucidation of nuclear structure and element-specific data more directly relevant to analytical applications. Data are handled differently for $A < 45$ than for heavier elements. While the database is readily available through the nuclear data centers, the data are voluminous and so structured as to be more useful to nuclear structure physicists rather than to scientists who wish to apply these data in PGAA. Many scientists find the compilation of thermal neutron capture γ-ray data by M.A. Lone and co-workers (published in 1981) to be more readily available. These valuable data, however, were measured twenty years ago in a single laboratory, are incomplete, and contain errors. An international effort is needed to create an up-to-date database with all the data needed for PGAA.

3. GENERAL RECOMMENDATIONS

The RCM found general agreement on the content of the database, and in outline agreed on the format of its presentation for users.

There are to be two databases: a working database (primarily for evaluators and nuclear structure physicists) which contains all the data, and an user oriented database derived from it, which contains evaluated data suitable for application to PGAA.

There was general agreement that the information produced by this CRP should be published in both electronic form and in an archival journal.

Existing isotope-specific data on levels and transitions in ENSDF will be combined with an extensive series of elemental measurements made with a thermal neutron guide in Budapest, other recent measurements, and data to be measured by participants in the CRP.

To ensure quality and to assess the effect of differing neutron spectra, the data need to be checked by measurements in laboratories involved in this CRP, particularly for those nuclides whose cross sections do not follow the 1/v law: Cd-113, Sm-149, Eu-151, Gd-155, and Gd-157. In a detailed discussion of neutron spectra, it was agreed that the IAEA would provide effective Westcott g-factors for those participants who provide the pointwise shape of the neutron energy spectrum.

Valuable comments and recommendations from Dr. Aslam Lone, the principal author of the best previous compilation, have been received by the Scientific Secretary. The group agreed with most of his suggestions about the formatting of the user tables. His comment that the only factor independent of the particular neutron source is gammas/capture is correct. However, the quantity that is most accurately measured is the ratio of counting rates of a γ-ray to that of a reference element. This is most effectively expressed in PGAA as in instrumental neutron activation analysis, as the k_0 factor: the product of capture cross section, isotopic abundance, and gammas per capture of the γ-ray divided by the same product for the reference gamma.

There was general agreement that authoritative, published sources of auxiliary data be used wherever appropriate, for example on Atomic Weights and Isotopic Abundances see the standards adopted by the International Union of Pure and Applied Chemistry (IUPAC), Pure Appl. Chem., 68, 2339-2359 (1996); 69, 2471-2473 (1997), (http://www.chem.qmw.ac.uk/iupac/AtWt/).

3.1 Recommended general database content and structure

- Nuclide specific
- Data sets for each nuclide from all available sources

- Best data set adopted

- ENSDF2 format
- γ-ray energy without recoil correction
- Neutron binding energy from fit to level scheme
- γ-ray intensity in authors units to preserve precision
  include systematic uncertainty
  normalisation to obtain γ-rays per 100 captures
- Cross-section information
  σ_o from Mughabghab most recent revision
  Westcott g-factor
- Isotopic abundance
- Half-life of decay species, isomers, and prompt levels
- Internal conversion coefficients
- General comments
- Detector, normalising factor, references, extent of energy balance
- Footnotes (if from different set, etc.)

3.2 Recommended application database with evaluated data suitable for use in PGAA

From the above described database, an object-oriented database will be constructed, appropriate for user applications, containing at least the following information:

- For each gamma line
  A, element name, E(keV), standard uncertainty, partial cross section (b), standard uncertainty, relative intensity, k_0, uncertainty, lifetime, standard uncertainty, flag for non-n, gamma reaction

- For each isotope
  A, element name, isotopic abundance, total neutron radiative capture cross section (b), uncertainty, Westcott g-factor, continuum component

- For each element
  Z, element name, atomic wt, σ_0

3.3 Experimental Facilities

Several experimental facilities are or will be available to the CRP, having different characteristics:

Budapest Neutron Center: Thermal guided beam, thermal equivalent flux $2x10^6$ cm^{-2} s^{-1} until now, soon to be replaced with a cold guided beam; anti-Compton and pair spectrometer

KAERI, Korea: Polychromatic diffracted beam, flux $1x10^8$
Dalat, Vietnam: Silicon filtered beam, flux $2x10^6$
BARC, India: Thermal guided beam, flux $2x10^7$

For additional information on the influence of neutron beam characteristics, it would be highly beneficial to bring more facilities into this program, in particular:

JAERI, Japan: Thermal and cold guided beams, using the same anti-Compton and pair spectrometer, $2x10^7$ and $1x10^8$ flux, respectively
NIST, USA: Thermal (sapphire filtered) and cold beams, $3\ x10^8$ and $8x10^8$ flux, respectively, with anti-Compton spectrometer.

3.4. Experimental Effort and Element Priorities

1. Spectroscopy benchmark
It is required that all participants perform a benchmark experiment involving
- acquisition of a prompt γ-ray spectrum
- fitting of γ-ray peaks
- relative efficiency calibration of detector
- determination of relative γ-ray intensities (strongest line = 100)

Selected target: titanium metal (and oxide).

2. Measurement of k_0 factors (partial cross-sections)
Concurrent determination of k_0 factors by using homogeneous composite targets containing the element of interest and an arbitrary comparator element in either of the following forms
- stoichiometric compound
- solution
- solid mixture

Priority list:
1. (H), B, C, N, P, Si, S, transition metals, Cd, Sm, Gd, Hg: important in analysis
2. Li, Ti, In, Ta, W, Tl, U-235: not well measured
3. He, Ne, Ar, Kr, Tc, Pm: not measured yet

3. Validation of k_0 method
The measured k_0 values have to be validated by measuring well-determined concentrations in
- certified reference materials
- artificial (homogeneous) mixtures
- alloys, cement

Priority list: see above

4. Development of correction procedures
To account for neutron and γ-ray absorption in voluminous samples, and for cross-section anomalies (non 1/v cases) it is necessary to develop easily applicable empirical correction procedures.
- Correction for absorption by using a reference element abundant in the matrix (Goswami)

- Effective Westcott g-factors determined for each facility separately (Cd, Sm, Eu, Gd, Hg)

4. ACTIONS TO BE TAKEN AS SOON AS POSSIBLE

1. Firestone and Zhou: Evaluate parameters for all elements and isotopes in ENSDF format, as described in Recommended evaluators database content and structure
2. Paviotti: Contact Mughabghab to obtain the status of the σ_0 evaluation, and make him aware of the possibility that this CRP may provide better values
3. Paviotti: Provide thermal g factors for database. (Done: INTER calculations on ENDF-VI Rev 3. Check if possibility of update new calculations)
4. Choi, Goswami, Molnár, Tan: measure and validate k_0 factors of elements in priority list
5. Lindstrom and Molnár create a reference material for neutron beam characterisation
6. Molnár: provide write-up of spectrometer calibration and distribute titanium specimens for benchmark measurement
7. Molnár: provide spectra to Victor Zerkin for display & overlay software development
8. Firestone: draft structure of object oriented database for discussion by next meeting
9. Lindstrom: distribute blind reference materials for validating k_0 method and evaluate results

5. INDIVIDUAL TASKS

Heedong Choi
Department of Nuclear Engineering
Seoul National University
Korea
Project Title: **Evaluation and measurement of k_0-factor for light elements of A<45**
Starting date of the project: 01/05/99

Programme of Work for the First year:

1. Calculation of k_0-factors for nuclides of A<45:
   chlorine comparator - done
   balancing check - to be done
2. Evaluation of gamma intensity data:
   completeness check - done
   balancing check - to be done

3. Study of correction factors for non-1/v absorbers:
   Westcott g-factors - done
   Neutron Temperature and other effects to be done
4. Qualification of comparator to be done
5. Make the data available to the IAEA/NDS.

6. Prepare report describing the work performed

Richard B. Firestone
Lawrence Berkeley National Laboratory
University of California
Berkeley, USA
Project Title: **Design of a Database for Prompt γ-Ray Neutron Activation Analysis**
Starting date of the project: 01/05/99

Programme of Work for the First year:
1. Evaluate isotopic (n, γ) data for Z=1-9 in co-ordination with Chunmei Zhou. Provide ENSDF format data sets checked for energy and intensity balance. Normalise intensity to per 100 neutron captures
2. Compile elemental (n, γ) into ENSDF format, isotopic data sets and check for energy and intensity balances.
3. Combine isotopic and elemental data into an adopted elemental database containing Eγ, dE_γ, I_γ (partial γ-ray production cross section), dI_γ, ICC, Abundance, Atomic Weight, and k_o
4. Develop PGAA Internet site containing description of the PGAA technique, links to PGAA activities, reference lists, and access to PGAA database.
5. Develop a PGAA search site and the WWW in collaboration with L. P. Ekstrom, Lund University. This site would be comparable to the WWW Table of Radioactive Isotopes.
6. Make the data and web software available to the IAEA/NDS.
7. Prepare report describing the work performed

A. Goswami
Nuclear Chemistry Section
Radiochemistry Division
BARC, Mumbai, India.
Project Title: **Evaluation and Measurement of prompt k_0**
Starting date of the project: 01/06/99

Programme of Work for the First year:
1. Compilation of prompt k_0 factors using existing data on thermal neutron capture cross sections and γ-ray abundances.
2. Experimental determination of prompt k_0 factors for a few select light elements (up to A=45) like H, B, C, N, Na, Mg, Al, Si, P, S, Cl and K.
3. Comparison of experimental and compiled data.

4. Checking of prompt k_0 factors by determining the constituents in special samples (NIST SRM 1571 and IAEA V-10) by k_0.
5. Make the data available to the IAEA/NDS.
6. Prepare a report describing the work performed.

Gábor L. Molnár
Institute of Isotope and Surface Chemistry,

Chemical Research Center
Budapest, Hungary
Project Title: **Capture γ-ray data for PGAA Database**
Starting date of the project: 01/04/99

Programme of Work for the First year:

1. Completion of measurements aimed at the improvement of elemental data for 14 elements (Ca, Co, As, Mo, Ru, Sn, I, Ho, Tb, Lu, Hf, Ta, W, Re), to obtain a high-quality spectrum library for all naturally occurring elements, except the noble gases.
2. Completion of internal standardisation measurements using stoichiometric (Cl-, H- or N-) compounds for the remaining 15 elements (Ga, Ge, Se, Ru, Rh, In, Ce, Tb, Ho, Tm, Lu, Hf, Ta, Re, Os) in order to deduce the normalising factors with respect to the H(n,γ) cross-section.
3. Determination of partial γ-ray production cross sections for all analytically important γ-ray transitions for 79 elements, from H to U.
4. Publication of the catalogue of spectra and γ-ray data as an LBNL report (in collaboration with R. B. Firestone)
5. Make the data available to the IAEA/NDS.
6. Prepare a report describing the work performed.

Vuong Huu Tan
Vietnam Atomic Energy Commission
Hanoi, Vietnam
Project Title: **Measurement of k_0 factors for some elements in prompt--ray neutron activation analysis**
Starting date of the project: 01/06/99

Programme of Work for the First year:

1. Standardization and characterisation of the PGAA facility at the Dalat reactor for k_0 factor measurements.
2. Measurements of k_0 factors in stoichiometric compounds relative to the 1951 keV γ-ray of Cl for the elements: B, C, N, Si, S, Cd, Gd, Sm, Hg.
3. Make the data available to the IAEA/NDS.
4. Prepare a report describing the work performed.

C. Zhou
China Nuclear Data Center
China Institute of Atomic Energy
Beijing, P. R. China
Project Title: **Evaluation of prompt γ-ray energies and absolute intensities for thermal neutron capture for nuclides with mass number A<45**
Starting date of the project: 01/04/99

Programme of Work for the First year:

1. Evaluation of γ-ray energies and intensities of thermal-neutron capture for nuclides with mass number A=1-25
2. Prepare data in the ENSDF format to be included in this library
3. Make data available to the IAEA/NDS
4. Report describing the work performed

6. CONCLUSIONS

PGAA has proved and will continue to prove to be a useful method of chemical analysis, which has been hampered by incomplete and out-of-date information. Significant progress has already been made at the beginning of this CRP in designing a definitive database and providing experimental verification of the basic data in this technique. The tasks agreed to by the participants will accomplish these goals.

It would be highly desirable to include JAERI and NIST in the CRP, both of which have unique facilities and years of experience in the development and application of PGAA.
We recommend that the IAEA publicise the results of this CRP to relevant applications within the Agency, and consider providing technical support to Member States interested in using the database to pursue applications of PGAA.

The next CRP meeting should be held at Agency Headquarters, April or May 2001.

APPENDIX 1

International Atomic Energy Agency
First Research Coordination Meeting on
"Development of a Database for Prompt γ-ray Neutron Activation Analysis"

IAEA Headquarters, Vienna, Austria
2 to 4 November 1999
Meeting Room C0739

AGENDA

Tuesday, 2 November

09:30 - 10:30 Opening Session

- Introduction of participants
- Opening (D.W. Muir, Head, IAEA Nuclear Data Section)
- Election of Chairman and Rapporteur
- Discussion and Adoption of Agenda (Chairman)
- Scope of the CRP (Scientific Secretary, IAEA)

10:30 - 10:45 Coffee break

10:30 - 12:30 Presentations by Participants
(15' for each participant and 5' discussion)

- Evaluation and Measurement of k_0-factor for Light Elements of A<45
  H.D. Choi, Korea
- Evaluation of prompt γ-ray energies and absolute intensities for thermal neutron capture for nuclides with mass number A<45
  Z. Chunmei, China
- Design of a Database for Prompt γ-ray Neutron Activation Analysis
  R.B. Firestone, USA
- Capture γ-ray Data for PGAA Database
  G.L. Molnar, Hungary
- Evaluation and Measurement of Prompt k_0

  A. Goswami, India
- Measurement of k_0-factors for some Elements in Prompt-Gamma Neutron Activation Analysis
  V.H. Tan Vietnam

12:30 - 14:00 Lunch and Administrative/Financial Matters Related to Participants

14:00 - 15:00 Overview of Present Status of Data: Main "gaps" where Data are needed (Gabor L. Molnar)

15:00 - 15:30 A User's Perspective on Data Quality and Accessibility (Richard M. Lindstrom)

15:30 - 16:00 Coffee break

16:00 - 16:20 Interactive Visual Analysis of Remote/Local Nuclear Data (Viktor Zerkin)

16:20 - 17:30 The Isotope Project Server and Software Available to CRP Participants (Richard B. Firestone)

Wednesday, 3 November

09:00 - 12:30 General discussion about:
Contents and structure of database, experimental facilities and experimental procedures to be adopted by participants, priorities, necessity of other proposals/agreements, next meeting's date and place.

12:30 - 14:00 Lunch

14:00 - 18:00 Scope and Workplan of the CRP and Begin Drafting of the Meeting Report

- Detailed Scope
  * Goals and priorities
  * Expected products

- Detailed working plan
  * Distribution of responsibilities
  * Individual tasks
  * Conclusions and recommendations

Thursday, 4 November

09:00 - 12:30 Drafting the Meeting Report

-

12:30 - 14:00 Lunch

14:00 - 17:00 Concluding Session

- Discussion and Approval of the Meeting Report

APPENDIX 2

International Atomic Energy Agency

First Research Coordination Meeting on

"Development of a Database for Prompt γ-ray Neutron Activation Analysis"

IAEA Headquarters, Vienna, Austria, 2 - 4 November 1999

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APPENDIX 3

Co-ordinated Research Project (Opening: D.W. Muir)

"Development of a Database for Prompt γ-ray Neutron Activation Analysis"

Meeting to be held in IAEA, 2-4 November

General remarks about CRPs

- CRP is an IAEA project (IAEA defines scope and objectives, selects participants and co-ordinates the work)
- Participants should tailor their work to meet the CRP objectives, not vice versa
- CRP is a valuable mechanism unique to the IAEA

CRP general procedures

- Scientific & technical work towards well defined objective
- International collaboration and co-ordination, role of IAEA technical officer
- Normally one participating laboratory per country, significant participation of developing countries.
- Usually 3 meetings, chairman selected from among participants (Chairman may change from one meeting to the next)

CRP products

- IAEA wants to see in 3 years a well defined product (normally a database) which should be published in appropriate media (TecDoc, Web, CD-ROM, Archival Journals).
- Database products are distributed by IAEA cost-free upon request.

APPENDIX 4

Co-ordinated Research Project "Development of a Database for Prompt γ-ray Neutron Activation Analysis"

Objectives of the CRP

The overall objective of this CRP is to improve the accuracy and completeness of the data needed in PGAA in order to make possible the reliable application of this technique in fields such as materials science, chemistry, geology, mining, archaeology, environment, food analysis, medicine and other areas.

To achieve this objective we need to produce an internationally recognized database taking into account new measurements, evaluations or improvement of the data below:

- Capture γ-ray energies and absolute intensities for the dominant neutron capture isotope of each chemical element.
- Thermal and subthermal neutron-capture cross sections for dominant isotopes.
- Correction factors to account for cross section deviations from the 1/v law.
- k_0-factors for all elements.

The design of the database should be such that access and retrieval by users is easy and practical.

The new data should be known by the scientific community and general users, therefore it is expected that the following products will be produced:

- Electronic database for use in PGAA with user oriented accessibility profile.
- TECDOC document
- Printed version of the database in an international recognized journal.
- IAEA-NDS Worldwide Web online access.

The products and data produced trough this CRP will be given to the Agency for cost free distribution according to the policy of the organization

Purpose of this meeting

The purpose of this meeting is to discuss the individual proposals and exchange ideas within the framework of the CRP.

1) **What data should be included in the tables ?**
2) **What would be the best format (formats) to present the data in the tables?**
3) **Assign a priority to each element/nuclide ?**

This will allow us to build a list of tasks and responsibilities of participating laboratories in order to fulfil the specific research objectives and produce in time the expected research outputs of the CRP

APPENDIX 5

International Atomic Energy Agency

Information Sheet on a Co-ordinated Research Project (CRP)

1. **Title of CRP:** ***"Development of a Database for Prompt Gamma-ray Neutron Activation Analysis"***

2. **Background Situation Analysis**

The International Nuclear Data Committee, at its 1997 meeting in Vienna, strongly recommended that the Nuclear Data Section supports the update and new measurements of data needed in neutron-induced Prompt Gamma Activation Analysis (PGAA) (see "Minutes of the 21st meeting of the International Nuclear Data Committee, February 1997", INDC/P(97)-20). The technique of PGAA, which uses thermal and subthermal (cold) neutron beams, is widely applied in materials science, chemistry, geology, mining, archaeology, environment, food analysis, medicine and other areas. Acting up on this recommendation, the CRP on "Development of a Database for Prompt-Gamma Neutron Activation Analysis" is being initiated.

PGAA is a non-destructive radioanalytical method, capable of rapid or in situ simultaneous multielement analysis involving the entire Periodic Table, from hydrogen to uranium. Typically, twenty or more elements can be identified in a single sample. Besides the elemental concentrations, isotope ratios can also be determined in favourable cases. The increasing importance of PGAA and its broad range of applicability are evident and have been emphasised at many meetings related to this topic, e.g., TCM in Vienna, 4-7 May 1993 ("Use of neutron beams for low and medium flux research reactors: radiography and materials characterisation" IAEA-TECDOC-837).

The availability of high-quality guided (or filtered) thermal and cold neutron beams at high and medium flux research reactors has greatly facilitated the advancement of the PGAA method during the 1990s ("Ninth International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics"; Budapest, 8-12 October, 1996; Springer, 1997). At the same time the AGM on the "Co-ordination of the Nuclear Structure and Decay Data Evaluators' Network" held in Budapest, 14-18 October 1996 (INDC(NDS)-363) stated that "there is a need for a complete and consistent library of cold and thermal neutron capture gamma-ray and corresponding cross section data" and recommended the organization of a CRP on the subject.

Inaccuracy and incompleteness of the data available for use in PGAA are a significant handicap in the qualitative and quantitative analysis of complicated gamma spectra. Accurate and complete neutron capture gamma-ray energy and intensity data, are also important in other fields such as shielding calculations and space science. Moreover, limited evaluated data are available for cold neutron capture calculations and k_0 determination and a convenient standardisation method for Prompt Gamma Neutron Activation Analysis need to be established. More details on the present status of data can be found in the attachment.

An international effort is needed to assemble this new and unique database, containing in one source all the data needed for PGAA, including corresponding uncertainties.

3. Overall Objective

The overall objective of the CRP is to improve the accuracy and completeness of the data needed in PGAA in order to make possible the reliable application of this technique in fields such as materials science, chemistry, geology, mining, archaeology, environment, food analysis, medicine and other areas.

4. Specific Research Objective

The specific research objective of this CRP is to produce an internationally recognized database taking into account new measurements, evaluations or improvements of the data below:

- Capture gamma-ray energies and absolute intensities for the dominant neutron capture isotopes of each chemical element.
- Thermal and subthermal neutron-capture cross sections for dominant isotopes.
- Correction factors to account for cross section deviations from the 1/v law.
- k_0-factors for all elements.

5. Expected Research Outputs

- Electronic database for use in PGAA.
- Printed version of the database.
- TECDOC document.
- IAEA-NDS Worldwide Web online access.

6. Participants

In order to participate in the CRP each participant must enter into a Research Agreement or a Research Contract with the IAEA. Participants from developed countries (as defined by the IAEA) enter into Research Agreements. The only financial support received from IAEA under a

Research Agreement is transportation and per diem of the chief scientific investigator or his representative to attend periodic CRP meetings. Participants from developing countries (as defined by the IAEA) can enter into Research Contracts. Under a Research Contract, in addition to financial support to attend CRP meetings, the participant receives limited financial support for research (typically US$ 5000 per contract year). Research contracts are reviewed (based on annual reports) and, subject to approval by the Director General, renewed each year for the duration of the CRP.

7. Duration

The CRP will run for three years (1999- 2002).

8. Additional Information

Additional Information can be obtained from:

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Present Status of Data

Gamma-ray data

The most reliable and complete source of information for thermal neutron capture gamma-ray data for nuclides is the Evaluated Nuclear Structure and Decay Data File (ENSDF), produced in an international effort by expert evaluators. The 1998 version of ENSDF has been included in the CD-ROM supplement to the 8th edition of the Table of Isotopes [1]. Updates of data for mass chains are also available in printed form in the journal Nuclear Data Sheets, and for light nuclei (A<45) in the journal Nuclear Physics A.

References to the original papers are included in the section Nuclear Structure References (NSR), also available on line from the National Nuclear Data Center, Brookhaven and the IAEA Nuclear Data Section, Vienna. In addition, there is the old and most useful compilation of thermal neutron capture gamma-ray data done by M.A. Lone and co-workers [2].

Close examination of the aforementioned sources of information has led to the following conclusions.

- ENSDF contains (n,γ) data for *NUCLIDES*, i.e. for the individual isotopes of each chemical element.
- Neutron capture gamma-ray data for nuclei with mass number A<45 are missing from ENSDF since they have not been included explicitly in the original evaluations printed in Nuclear Physics A. Capture data for nuclides with mass number A>44 are systematically included in ENSDF but the normalisation of absolute gamma-ray intensity is often missing or ambiguous. In some cases only a subset of gamma rays is available. These may be the primary gamma rays, de-exciting the capture state directly, or the secondary gamma ray cascades from the levels fed by the primaries. The two have often been measured in a different experiment, or one of them not measured at all. Hence the data may be incomplete, or the intensities of both primary and secondary gamma rays may not be uniquely normalized. Tests for completeness have shown that gamma-ray data for only 22 nuclides out of the 217 cases may be considered satisfactory [3]. Obviously, there are too many missing gamma-ray transitions for most nuclei that affects the normalisation.
- References to original (n,γ) papers are included in NSR for all nuclei. Hence the missing data can be retrieved and evaluated.
- For *ELEMENTS*, the only compilation of thermal neutron capture gamma-ray data is that of Lone et al.[2], containing data which essentially come from a single series of over 25 years old measurements. In this pioneer and outstanding compilation, only the (fairly large) uncertainty ranges for energies are included while individual uncertainties of absolute gamma-ray intensities per 100 captures and elemental cross sections are missing. Lack of data for the important element uranium (Z=92) is also a deficiency. The IAEA has made these tables available on a floppy disk .

The Lone data for the light elements and ENSDF data from 1991 for the heavier nuclides

- (A>44) have recently been combined by Tuli [4] on a World Wide Web home page where gamma-ray energies and intensities (relative to 100 for the strongest transition) are provided without uncertainties.

Cross sections

Thermal-neutron cross sections, σ_0, (or values measured in a Maxwellian flux when unavailable) and resonance integrals, I_0, and evaluated neutron resonance parameters can be found in refs. [5,6] while experimental energy-differential cross section data are included in ref. [7]. The thermal neutron-capture cross sections and the resonance integrals have recently been recompiled by Holden [8]. Experimental cross sections from the actual CSISRS data file as well as evaluated cross section curves are accessible at various Web sites. Westcott g-factors are the simplest indicators of any deviation from the 1/v law. They have been calculated for the ENDF/B-V evaluation (see ref. [9]). More recent values, derived from JEF-2.2 data by the same INTER code, are available as part of the JEF-2.2 data files [10].

Problems:

- The precision of thermal neutron-capture cross sections [5,7] is quite diverse. There are only 14 nuclides, representing 12 chemical elements (H, Na, Cl, Co, Cu, In, La, Gd, Hf, Au, Th, U), for which the relative uncertainty is better than 1%. For another 19 nuclides it is between 1-2% while the majority of data fall in the uncertainty classes with 5%, 10% and 25% upper limits, respectively, with about equal population.
- Experimental capture cross sections for neutron energies below thermal (cold neutrons!) are available for a very limited number of nuclides. This is also true for most total cross sections. Therefore, cold-neutron cross sections have to be extrapolated to the desired neutron energy by using the evaluated set of neutron resonances, unless the 1/v law has been verified to apply.

Usefull resources in this field are World Wide Web home pages e.g:
http://www.iki.kfki.hu/nuclear/, from the Institute of Isotope and Surface Chemistry, Budapest; http://ie.lbl.gov/ng.html, from the Lawrence Berkeley National Laboratory; http://www-nds.iaea.org/indg_intro.html from the Nuclear Data Section, IAEA; http://www.nndc.bnl.gov/wallet/tnc/capgam.shtml, from Brookhaven National Laboratory http://iriaxp.iri.tudelft.nl/~rc/fmr/k0www/k0conten.htm from the Laboratory for INAA, University of Technology, The Netherlands; etc.

Standardisation factors

For neutron activation analysis (NAA) with a single comparator element (usually Au) a composite nuclear constant has been introduced which can be used to obtain elemental concentrations from the measured activities after co-irradiating sample and comparator. This

so-called k_0-factor is the product of isotopic abundance, (n,γ) cross section and absolute gamma-ray intensity per molar mass, related to a similar product for the comparator. The k_0-factors have been measured directly for over 100 radionuclides, in most cases with a precision of 1-2% or better [11]. Therefore, they can be used for checking the consistency of nuclear data involved or, whenever either cross section or intensity are precisely known, for deducing the other quantity. Indeed, new σ_0 values have been obtained by using experimental k_0-factors and absolute intensities per decay from ENSDF for 103 radionuclides [12-13]. It is possible to explore this concept in the following way:

- The NAA k_0-factors can be used to improve cross-section data, especially when a new set of evaluated decay data become available for the most important 200 radionuclides.
- The concept of k_0 standardisation has recently been extended to the PGAA case [14]. The prompt k_0-factors relative to Cl comparator are already measured for 16 nuclides [15] and they can be used to infer absolute gamma-ray intensities per capture, provided the thermal cross sections are precisely known and they obey the 1/v law.
- It should also be kept in mind that capture cross sections are to some degree reactor specific, because of the variations in mean neutron energy in neutron beams. However, this does not reduce the need for evaluated data compilations as long as the neutron energies are specified.

MAIN TASKS*:*

1. Evaluate capture gamma-ray data for light elements (A<45) to complete the ENSDF set.
2. Check the full set of capture gamma data for completeness, check normalisation of intensities.
3. Where there are discrepant thermal capture cross section data or evaluations, a re-evaluation of the data is to be carried out in order to be able to renormalise the gamma-ray intensities of the pertinent isotope.
4. Create database for isotopes (nuclides) containing gamma-ray energies and intensities from the isotopic ENSDF data.
5. For each element, compare the ENSDF data with newly measured elemental data, renormalise the intensities if necessary, and deduce a recommended set.
6. Make the new library available for users. (WWW, CD-ROM, IAEA Report).

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APPENDIX 6

Extended Abstracts of Technical Papers

Evaluation and Measurement of Prompt k_0-factor for Light Elements of A < 45

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1. Calculation of the Prompt k_0-factors

Prompt k_0-factors for light elements (A<45) are calculated by using absolute gamma intensity data for isotope from LBNL (Lawrence Berkeley National Laboratory, USA)-IKI(Institute for Isotope, Hungary)[1] and absolute gamma intensity data for element from Lone table[2], respectively. The chlorine is adopted as comparator. The products are tabulated in the World Wide Web[3]. In Fig. 1, the calculated values are shown in comparison with the measured data by Moln r et al.[4] for several elements. The values obtained by using Lone table deviate relatively large. Those values by using LBNL-IKI data are consistent closely, where the k_0 values for ^{1}H, ^{23}Na, ^{40}K and ^{44}Ca are consistent within 10% while that for ^{12}C is not consistent.

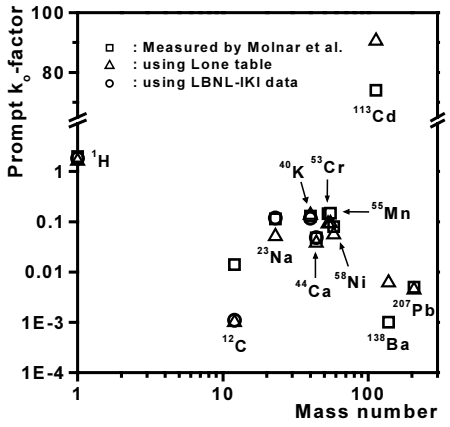

Fig. 1. Comparison between the measured and the calculated prompt k_o-factor for some isotopes.

2. Consistency of the Absolute Gamma Intensity Data

To check the consistency between the measured and the calculated prompt k_0-factors in detail, it is necessary to evaluate the absolute gamma intensity data of large uncertainty. We exploited the fact that the sum of all transition energies multiplied by the absolute gamma intensities equals the Q-value of the (n, γ) reaction. Fig. 2. shows that LBNL-IKI intensity has a fair consistency with the Q-value based on Audi masses[5]. Recoil energy correction makes slight difference for the light isotopes. The checking of feeding and decaying intensities for the relevant levels is going on.

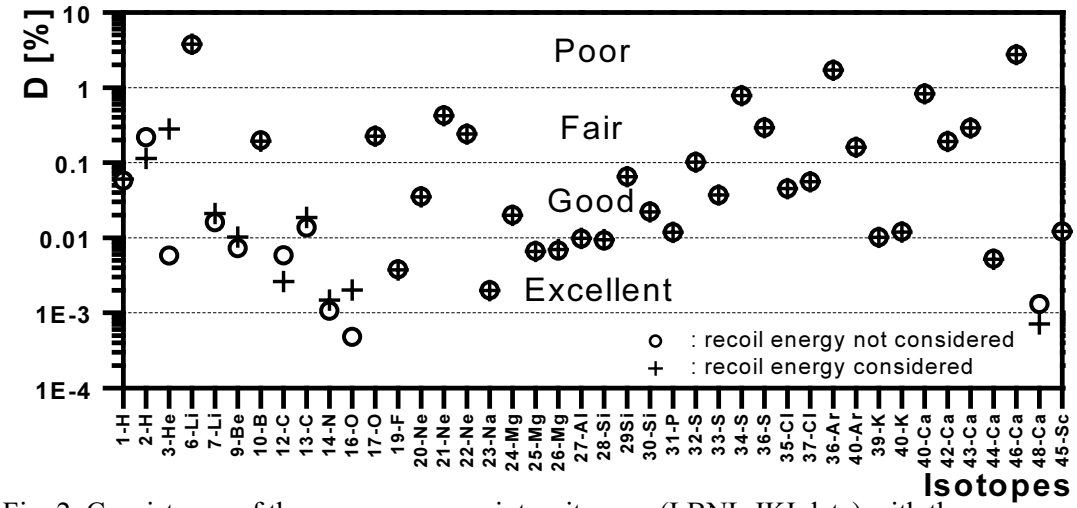

Fig. 2. Consistency of the gamma energy-intensity sum (LBNL-IKI data) with the Q-value (The criteria of Excellent, Good, Fair or Poor are arbitrary.)

3. Experimental Correction Factor of the Prompt k_0-factors

The PGNAA system being constructed at HANARO research reactor at Korea Atomic Energy Research Institute(KAERI) is going to use a polychromatic thermal neutron beam diffracted by pyrolytic graphite(PG) crystal. For this type of spectral neutron beam, a correction factor Ω in the measurement of prompt k_0-factors is required for non-1/v absorbers and is given by

$$\Omega = \frac{\sum_k \omega_s(E_k)\phi_k / \nu_k}{\sum_k \omega_c(E_k)\phi_k / \nu_k} \qquad (1)$$

where $\omega(E_n) = \sigma(E_n)\nu_n / \sigma_0\nu_0$. The Ω-factor is reduced to a ratio of Westcott g-factors for Maxwellian neutron spectrum. In Fig. 3, the Ω-factor is compared with Westcott g-factor ratios between those of the comparator and the standard. The Westcott g-factor ratios are close to 1 for the isotopes of 1/v cross section, but deviate largely from 1 for ^{113}Cd due to non-1/v cross section. The Ω-factors are about 1 for all isotopes including ^{113}Cd. Hence the discrete neutron spectrum will be good for measuring prompt k_0-factors of non-1/v absorbers.

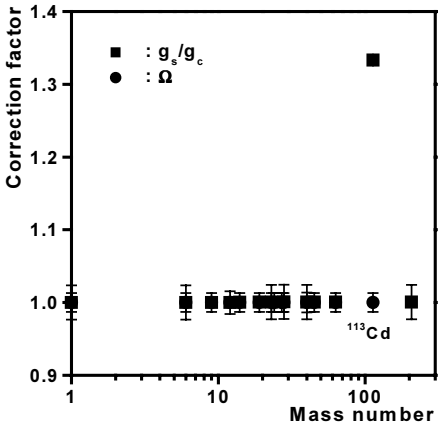

Fig. 3. Correction factor for various isotopes.

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Error Assignment of g(T)

$$g = g(T) = \frac{1}{s_0 v_0}\int_0^\infty \frac{4}{\sqrt{p}}\left(\frac{v}{v_T}\right)^3 e^{-(v/v_T)^2} s(v)dv, \quad (1)$$

$$\Phi_M(v) = \frac{4}{\sqrt{p}}\left(\frac{v}{v_T}\right)^3 e^{-(v/v_T)^2}, \quad (2)$$

where s_0 is the 2200 m/sec cross section, v_0 = 2200 m/sec, v_T is the most probable velocity of the Maxwellian density distribution. If we assume that the random errors are associated with s_0 and $s(v)$ in the calculation of g-factor, the propagation of errors gives

$$dg = g - \bar{g} = \frac{1}{s_0 v_0}\int_0^\infty \Phi_M(v) ds(v) dv - \frac{ds_0}{s_0^2 v_0}\int_0^\infty \Phi_M(v) s(v) dv \quad (3)$$

$$= \frac{1}{s_0 v_0}\int_0^\infty \Phi_M(v) ds(v) dv - g\cdot\frac{ds_0}{s_0}, \quad (4)$$

where d denote the random variation, -(bar) is the statistical expectation value. By changing the variable of integration $x = v/v_T$,

$$\frac{1}{s_0 v_0}\int_0^\infty \Phi_M(v) ds(v) dv = \frac{v_T}{s_0 v_0}\int_0^\infty \Phi_M(x) ds(x) dx, \quad (5)$$

$$\Phi_M(x) = \frac{4}{\sqrt{p}} x^3 e^{-x^2} \quad (6)$$

and $$dg = \frac{v_T}{s_0 v_0}\int_0^\infty \Phi_M(x)ds(x)dx - g\cdot\frac{ds_0}{s_0}, \tag{7}$$

$$(dg)^2 = \left(\frac{v_T}{s_0 v_0}\right)^2\left[\int_0^\infty \Phi_M(x_1)ds(x_1)dx_1\right]\left[\int_0^\infty \Phi_M(x_2)ds(x_2)dx_2\right] + g^2\cdot\left(\frac{ds_0}{s_0}\right)^2$$

$$-2g\cdot\frac{v_T}{s_0^2 v_0}ds_0\int_0^\infty \Phi_M(x)ds(x)dx \tag{8}$$

$$= \left(\frac{v_T}{s_0 v_0}\right)^2\int_0^\infty\int_0^\infty \Phi_M(x_1)\Phi_M(x_2)ds(x_1)ds(x_2)dx_1dx_2$$

$$-2g\cdot\frac{v_T}{s_0^2 v_0}\int_0^\infty \Phi_M(x)ds(x_0)ds(x)dx + g^2\cdot\left(\frac{ds_0}{s_0}\right)^2, \tag{9}$$

where $ds(x_0)\equiv ds(v_0) = ds_0$.

$$\mathrm{var}(g) = E\{(dg)^2\} = \left(\frac{v_T}{s_0 v_0}\right)^2\int_0^\infty\int_0^\infty \Phi_M(x_1)\Phi_M(x_2)E\{ds(x_1)ds(x_2)\}dx_1dx_2$$

$$-2g\cdot\frac{v_T}{s_0^2 v_0}\int_0^\infty \Phi_M(x)E\{ds(x_0)ds(x)\}dx + g^2\cdot E\left(\frac{ds_0}{s_0}\right)^2. \tag{10}$$

Here $E\{ds(x_1)ds(x_2)\} = E\{ds(v_1)ds(v_2)\} = \mathrm{cov}(s(v_1), s(v_2))$

and $E\{ds(x_0)ds(x)\} = E\{ds(v_0)ds(v)\} = \mathrm{cov}(s(v_0), s(v))$.

If the detailed information about the correlation between the cross section for different velocities is not known, hence there is no way but to assume $s(v)$'s are all independent for different velocities, one can see

$$\mathrm{cov}(s(v_1), s(v_2)) = \mathrm{var}(s(v_1))d_D(v_1 - v_2), \tag{11}$$

where $d_D(v_1 - v_2)$ is the Dirac delta function.

Then

$$\mathrm{var}(g) = \left(\frac{v_T}{s_0 v_0}\right)^2 \int_0^\infty \int_0^\infty \Phi_M(x_1)\Phi_M(x_2)\,\mathrm{var}\left(s(x_1)\right) d_D(x_1 - x_2)\,dx_1 dx_2$$

$$- 2g \cdot \frac{v_T}{s_0^2 v_0} \int_0^\infty \Phi_M(x)\,\mathrm{var}(s(x)) d_D(x - x_0)\,dx + g^2 \cdot \frac{\mathrm{var}(s_0)}{s_0^2} \qquad (12)$$

$$= \left(\frac{v_T}{s_0 v_0}\right)^2 \int_0^\infty \Phi_M{}^2(x_1)\,\mathrm{var}\left(s(x_1)\right) dx_1$$

$$- 2g \cdot \frac{v_T}{s_0^2 v_0} \Phi_M(x_0)\,\mathrm{var}(s(x_0)) + g^2 \cdot \frac{\mathrm{var}(s(x_0))}{s_0^2}. \qquad (13)$$

$$= \left(\frac{v_T}{s_0 v_0}\right)^2 \int_0^\infty \Phi_M{}^2(x)\,\mathrm{var}\left(s(x)\right) dx + \frac{\mathrm{var}(s(v_0))}{s_0^2}\left\{g^2 - 2g \cdot \frac{v_T}{v_0} \cdot \Phi_M(x_0)\right\} \qquad (14)$$

(and $\Phi_M(x_0) = \frac{4}{\sqrt{p}} \cdot \left(\frac{v_0}{v_T}\right)^3 e^{-(v_0/v_T)^2}$)

$$= \left(\frac{v_T}{s_0 v_0}\right)^2 \int_0^\infty \Phi_M{}^2(x)\,\mathrm{var}\left(s(x)\right) dx$$

$$+ \frac{\mathrm{var}(s(v_0))}{s_0^2} \cdot g\left\{g - \frac{8}{\sqrt{p}}\left(\frac{v_0}{v_T}\right)^2 e^{-(v_0/v_T)^2}\right\}. \qquad (15)$$

This approach requires the functional form for the variance of cross section $\mathrm{var}(s(v))$. If there is only discrete variances are available for specific values of v, i.e. $v_1, v_2, \cdots, v_n$, one can only approximate the integration in terms of the known uncertainties for $s(v_n)$'s by such as Gaussian quadrature. If there is no variance value

available for the integration but an estimate of $\mathrm{var}(\sigma(v))$ as a constant $\mathrm{var}(\sigma)$ independent of the neutron velocity, the first integration is given by

$$\left(\frac{v_T}{\sigma_0 v_0}\right)^2 \int_0^\infty \Phi_M{}^2(x)\,\mathrm{var}(\sigma(x))dx = \left(\frac{v_T}{\sigma_0 v_0}\right)^2 \mathrm{var}(\sigma)\int_0^\infty \Phi_M{}^2(x)dx = \left(\frac{v_T}{\sigma_0 v_0}\right)^2 \mathrm{var}(\sigma)\frac{1}{\pi\sqrt{2}}\Gamma(\tfrac{7}{2})$$

$$= \frac{1}{\sqrt{2\pi}}\frac{15}{8}\left(\frac{v_T}{v_0}\right)^2 \frac{\mathrm{var}(\sigma)}{\sigma_0^2}\ .$$

Prompt gamma-ray data evaluation of thermal-neutron capture for A=1-25

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The method of prompt gamma-ray data evaluation for thermal-neutron capture has been briefly presented. The prompt capture gamma-ray data of stable nuclei for A=1-25 are evaluated. The evaluated data have been changed into the ENSDF format and the checks of physics and format have been made.

1 Main evaluation programs and their function

Main programs of thermal-neutron capture prompt gamma-ray data evaluation and their functions are listed in Table 1. These codes are mainly from Interna tional Network of Nuclear Structure and Decay data Evaluation, the ENSDF data format is adopted in these data evaluation.

Table 1, Main codes and their functions of prompt gamma-ray data evaluation for thermal-neutron capture

Code name	main functions
GTOL	level energy calculation by fitting to gamma-energies; intensities balance calculation & checking
LWA	limit-weighted and unweighted averages of measured data
HSICC	internal conversion coefficients calculation
HSMRG	format conversion from free format to ENSDF format
RADLST	energy balance calculation & checking
FMTCHK	ENSDF data format checking
PANDOR	ENSDF physics checking
ENSDAT	drawing decay schemes & listing data tables

2 Process of prompt neutron capture gamma data evaluation

The main process of thermal-neutron capture gamma-ray data evaluation is as follows:

a, Measured data collection

An evaluator retrieves related references from Nuclear Science References File, NSRF. On the basis of the retrieval, all measured data are collected from journals, reports, and private communications.

b, Measured data evaluation and recommendation of the best measured data

Gathered all related-data are analyzed and compared, treated by mathematical method (for example, weighted or unweighted averages of measured data). And then, the best-measured data and decay scheme can been recommended on the basis of the measured data evaluation.

c, Establishment of temporary data file

After recommendation of the best-measured data, the evaluated data are put into

computer by hand, the temporary data file can been set up in ENSDF data format.

d, Theoretical calculation

Format checking have been done for temporary data file, and correction to old one must be done if necessary. After then, Physics analysis and theoretical calculation are done and calculation results will be put into the gapes with no measured data so that recommended data become a self-consistent and complete data set.

e, Recommendation of complete data set

The above-complete data set of thermal-neutron capture prompt gamma-ray data and its decay scheme is recommended as evaluated data set.

f, checking

Physics and format checking has been done and correction must be done if necessary. Specifically, checking of intensity balance must be done. The adjustment should be done if necessary. The condition of the balances is as follows:

A nucleus captures a neutron and becomes a compound-nucleus. And then, It decays in emitting gamma-ray and conversion-electron. If a level scheme is complete and internal conversion can be neglected, the primary-ray intensities of captured state and secondary-ray intensities to ground state should all be the same within their uncertainties.

3 Data evaluation situation

The prompt gamma-ray data and their decay schemes of thermal-neutron capture for stable nuclei ^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{12}C, ^{13}C, ^{14}N, ^{16}O, ^{17}O, ^{19}F, ^{20}Ne, ^{21}Ne, ^{22}Ne, ^{23}Na, ^{24}Mg, and ^{25}Mg have been evaluated by using these programs. The evaluated data have been changed into ENSDF format and checked in Physics and ENSDF format.

IAEA Coordinated Research Project on the Development of a Database for Prompt Gamma-Ray Neutron Activation Analysis

Progress Report

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The design of a PGAA database has begun at the Lawrence Berkeley National Laboratory. The primary goals of this project are:

1. Design the content and structure of the PGAA database
2. Develop software for the evaluation of PGAA data.
3. Provide Internet dissemination tools to the CRP members and the IAEA/NDS.
4. Make neutron capture data from the Evaluated Nuclear Structure Data File (ENSDF) available to CRP participants and the IAEA/NDS.
5. Prepare a report describing the work performed.

PGAA Database Design

We have determined that the PGAA database should contain prompt gamma-ray energies, cross-section yields, and k0 factors for all elements for both cold and thermal neutrons. In addition, data for isotopic abundance, thermal neutron cross sections, and g-factors, are required. Also, gamma-ray data for short-lived radioisotopes produced by neutron activation should be included with the PGAA database. It also is desirable to maintain a database of elemental PGAA gamma-ray spectra.

The final PGAA database will combine the results of elemental capture data, where k0 factors are usually best determined, with ENSDF data which is derived mainly from isotopic capture data. The ENSDF data often contains more complete gamma-ray data than the elemental measurements. These data will be combined into ENSDF format files where level-scheme energy and intensity balance constraints can be applied to test the data. We expect to develop the PGAA database in ENSDF format and derive an object-oriented database from the ENSDF source for applied use.

Software Development

Several Windows/PC computer codes are available for evaluating the ENSDF format PGAA data. The computer code ENDIT has been developed for editing the PGAA datasets. The code ICC is used to calculate internal conversion coefficients. GAMUT is used to fit level energies and combine multiple measurements of gamma-ray energies and intensities. The code BALANCE determines the intensity balance through the level scheme. In addition, the code NGMATCH was developed to compare the elemental measurements with ENSDF. These programs will be made available to participants in the CRP and the IAEA/NDS.

Dissemination Tools

The Isotope Project develops nuclear data dissemination tools and maintains an Internet server. Isotope Explorer was developed as a helper application for viewing nuclear structure and decay data. This software is distributed, at no cost, over the Internet at http://ie.lbl.gov/toi.html and on the Table of Isotopes CD-ROM. We also provide a Capture Gamma home page at http://ie.lbl.gov/ng.html. The home page contains capture gamma data from the Lone tables and ENSDF, energy-ordered gamma-ray tables from both sources, thermal neutron cross sections from Mughabghab, and isotopic abundances by De Bievre. The group also maintains the WWW Table of Radioactive Decay database in collaboration with Lund University, Sweden at http://nucleardata.nuclear.lu.se/nucleardata/toi/. This database supports data searches and display of spectra.

The ENSDF format PGAA database will be made available on through Isotope Explorer and from the Capture Gamma home page over the Internet. We have been asked by researchers in PGAA to prepare a PGAA homepage and we will present a prototype of this page at the CRP meeting. This page will contain a description of the PGAA method, links to references and places were PGAA research is performed, and links to the available PGAA data. We encourage the participants in this CRP to develop individual Internet pages describing their activities. The Isotopes Project will be happy to assist in developing and hosting these pages. Our plan is to develop a WWW PGAA Database with Lund to disseminate the object-oriented form of the PGAA database.

ENSDF Neutron Capture Data

The ENSDF database was developed as a nuclear structure database with less emphasis on applications. It consists of an adopted level and gamma-ray dataset for each isotope, and a variety of additional reaction and decay datasets including neutron capture. These neutron capture datasets are traditionally evaluated to determine nuclear level properties, so the gamma-ray intensity normalizations are often incomplete. The ENSDF file does not contain thermal neutron cross sections or isotopic abundances. Thus, it is not possible to calculate k0 factors directly from ENSDF.

We have begun a systematic re-evaluation of the thermal and cold neutron capture data in ENSDF. We are updating the file with newer references, and cross sections and abundances are being added. Data from multiple experiments are combined using the GAMUT code, corrections for internal conversion are added using ICC, and the intensity balance through the level scheme is checked using BALANCE. We have evaluated Z=1-21 and these data are currently available on the Neutron Capture home page. With help from other CRP members we could complete the ENSDF format evaluation for all elements by the end of the CRP.

New Capture Gamma-ray Data for PGAA Database

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Abstract

A new catalogue of prompt gamma rays has been created on the basis of experiments at the Budapest PGAA facility. It contains elemental spectra and a table with nearly 7000 gamma rays with relative intensity over 1 percent of the strongest line. The average accuracy is about 0.08 keV for energies and about 5 percent for cross-sections in the whole energy range, from about 40 keV to 11 MeV.

Neutron induced prompt γ-ray activation analysis (PGAA) is based on the observation of instantaneous gamma radiation following the neutron reaction, which is mostly radiative capture, usually denoted as (n,γ) reaction. The energies of the emitted γ rays are characteristics of the element (more precisely, its radiating isotope), whereas the corresponding spectral intensities are proportional to the elemental content. In a prompt spectrum, however, the very large number of peaks (order of 1000) tremendously increases the chance for spectral interference. Hence, a suitable analytical library must contain very precise energy and γ-ray production cross-section data for all stable elements (and preferably their main isotopes). From such a library the analytical sensitivities could also be derived with confidence for any PGAA facility. Unfortunately, the currently available databases are incomplete, and contain many inconsistent and imprecise data. Moreover, they do not provide directly the γ-ray yields (or more precisely, the γ-ray production cross-sections) or, alternatively, the k_0 factors needed for the determination of elemental concentrations without applying any standards.

A new catalogue of subthermal neutron-induced prompt gamma rays has been created for 79 elements, from hydrogen to uranium (including fission), on the basis of recent measurements at the Budapest guided-neutron PGAA facility [1]. New energy values have been measured using ^{35}Cl neutron-capture gamma rays, while the gamma-ray production cross sections and k_0 factors have been determined as described below. The elemental data have been compared with thermal neutron-capture data for individual nuclides from the Evaluated Nuclear Structure Data File, ENSDF [2], hence isotope identifications could also be made.

The γ ray production cross-section is the product of isotopic abundance, θ, γ-ray intensity per capture, I_γ, and neutron capture cross-section, σ, i.e.,

$$\sigma(E_\gamma) = \theta \cdot I_\gamma \cdot \sigma \qquad (1)$$

It is measured in the usual b (barn) units, where 1 b = 10^{-28} m^2. For nuclides obeying the *1/v* law the reaction rate does not depend on the velocity of the neutron, hence σ can be replaced with the 2200 m·s^{-1} thermal cross-section, σ_0. The thermal-equivalent $\sigma(E_\gamma)$ values have been determined by us directly using the 0.3326±0.0007 b thermal capture cross-section [3] and the

(99.985±0.001)% isotopic abundance [4] for ^{1}H, which produces only one capture γ ray and serves as a convenient standard (see Révay et al., [5]).

When mass fractions or mass ratios are determined, the prompt k_0 factor [6] is usually preferred [7]. This is simply the ratio of $\sigma(E_\gamma)$ values for analyte, *x*, and comparator, *c*, both related to their corresponding molar mass, i.e.,

$$k_{0,c}(x) = \frac{\theta_x I_{\gamma x} \sigma_x / M_x}{\theta_c I_{\gamma c} \sigma_c / M_c} \qquad (2)$$

Hence the k_0 values can easily be calculated for any γ ray with respect to an arbitrary comparator. They are given for 164 strong, interference-free γ rays of 79 elements altogether in Table 1, after ref. [5].

The resulting database contains nearly 7,000 γ rays for 79 naturally occurring elements from H to U, which corresponds to almost 100 lines per element on the average. Table 2 is an excerpt from the new prompt γ-ray catalogue. It shows the new data side by side with the ENSDF energies and isotope labels. In the Comment column we indicate whether the γ ray originates from a different reaction, e.g., (n,α) or (n,f), or from a decay with the indicated half-life. Beside the relative intensity (strongest = 100 for each element), the directly measured γ-ray production cross-section, $\sigma(E_\gamma)$, is given to facilitate the determination of elemental concentrations.

To assess the degree of improvement over older data, the γ-ray production cross-sections inferred from the Lone table [8] have been compared with our directly measured values for 164 strong transitions in 79 elements [5]. The production cross-sections from Lone have been obtained for each γ ray by multiplying the intensity per capture with the capture cross-section given in their table. The ratios of Lone to Budapest cross-sections have been plotted as a histogram according to 0.2-wide ratio bins. It is striking that 39 of the 164 selected γ rays are missing entirely from the Lone table. Besides, only a fraction of cases (i.e., 48) fall in the two central bins with upper limits of 1.0 and 1.2, respectively. A much better agreement would be expected from the estimated upper limit of ±20% for the relative standard uncertainty of γ-ray intensity per capture [9].

In conclusion, the new catalogue of neutron-induced prompt γ rays, resulting from a series of measurements on a thermal neutron guide at the 10-MW Budapest Research Reactor, is complete enough to encompass all the important chemical elements occurring in nature. Moreover, it includes the frequently assayed isotopes D and ^{235}U separately. Intense prompt γ rays from the ^{10}B(n,α)^{7}Li and ^{235}U-fission reactions, as well as decay γ rays from short-lived reaction products have also been determined. The average accuracy is about 0.08 keV for energies and about 5 percent for cross-sections in the whole energy range, from about 40 keV to 11 MeV.

Table 1. Prompt k_0 factors determined at Budapest

Z	El	A	E keV	unc. keV	k_0(H)	unc. %
1	H	1	2223.26	0.02	1	0.2
1	H	2	6250.2	0.1	1.48E-05	5
3	Li	6	7246.8	0.3	9.19E-04	8
3	Li	7	2032.31	0.07	1.74E-02	5
4	Be	9	6809.6	0.1	1.78E-03	9
4	Be	9	3367.48	0.04	5.87E-04	9
5	B	10	477.60[d]	5.00[d]	2.00E+02	0.3
6	C	12	1261.71	0.06	3.10E-04	2.7
6	C	12	4945.30	0.07	6.81E-04	2.9
7	N	14	1884.85	0.03	3.14E-03	1.3
8	O	16	2184.38	0.04	3.20E-05	15
8	O	16	870.68	0.03	3.31E-05	6
9	F	19	583.49	0.02	5.62E-04	4.3
9	F	19	1633.60[e]	0.02	1.53E-03	4.3
11	Na	23	472.22[f]	0.01	6.55E-02	1.5
11	Na	23	90.98	0.02	3.28E-02	2.0
12	Mg	24	584.94	0.02	4.03E-03	4.7
12	Mg	25	1808.62	0.06	2.31E-03	4.7
13	Al	27	7723.8	0.3	7.53E-03	2.0
13	Al	27	1778.85[g]	0.03	2.62E-02	1.3
14	Si	28	3538.98	0.05	1.28E-02	1.7
14	Si	28	4933.83	0.07	1.22E-02	2.0
15	P	31	636.57	0.02	3.03E-03	5
16	S	32	841.01	0.01	3.37E-02	1.7
16	S	32	5420.24	0.1	2.92E-02	4.0
16	S	34	4637.5	0.1	7.12E-04	3.0
17	Cl	35	517.08	0.02	6.74E-01	1.5
17	Cl	35	786.24	0.02	3.04E-01	1.5
17	Cl	35	788.37	0.02	4.70E-01	1.5
17	Cl	35	1164.83	0.01	7.86E-01	1.5
17	Cl	35	1951.15	0.02	5.55E-01	0.8
17	Cl	35	1959.32	0.02	3.62E-01	1.2
17	Cl	37	4414.8	0.2	8.44E-03	8
17	Cl	35	6110.64	0.14	6.11E-01	8
19	K	39	770.33	0.02	7.06E-02	1.3
19	K	41	107.08	0.03	2.5E-03	1.9
20	Ca	40	1942.68	0.03	2.58E-02	3.0
20	Ca	43	1156.87	0.06	6.41E-04	3.9
20	Ca	44	174.01	0.09	1.23E-03	4.0
21	Sc	45	584.80	0.03	1.23E-01	1.9
22	Ti	47	983.50	0.03	7.23E-03	1.5
22	Ti	48	1381.74	0.03	3.28E-01	2.3
22	Ti	49	1553.80	0.04	6.05E-03	2.1
23	V	51	125.23	0.03	9.58E-02	3.0
23	V	51	1434.06	0.01	2.94E-01	2.1
24	Cr	50	749.10	0.03	3.32E-02	2.0
24	Cr	52	7937.86	0.12	2.47E-02	2.5
24	Cr	53	834.80	0.03	8.04E-02	2.5
25	Mn	55	846.75[h]	0.02	7.08E-01	1.2
26	Fe	54	9297.9	0.2	4.21E-03	3.3
26	Fe	56	352.33	0.02	2.78E-01	3.0
26	Fe	56	7631.05	0.09	3.74E-02	1.9
26	Fe	56	7645.49	0.09	3.17E-02	2.5
26	Fe	57	810.71	0.03	1.49E-03	4.0
27	Co	59	229.81	0.02	3.69E-01	1.2
27	Co	59	555.94	0.02	1.53E-01	1.2
28	Ni	58	464.97	0.02	4.35E-02	2.0
28	Ni	58	8998.31	0.09	7.69E-02	2.0
28	Ni	60	7819.55	0.08	1.74E-02	2.0
28	Ni	62	6837.44	0.06	2.37E-02	2.0
29	Cu	63	277.99	0.03	4.61E-02	2.0
29	Cu	63	7915.00	0.09	4.49E-02	2.0
29	Cu	65	185.66	0.03	1.26E-02	3.0
29	Cu	65	1039.2	0.2	3.22E-03	3.0
30	Zn	64	115.26	0.02	7.79E-03	3.0
30	Zn	66	6958.45	0.12	1.94E-03	8
30	Zn	67	1077.34	0.02	1.71E-02	1.4
30	Zn	68	1007.81	0.03	2.60E-03	2.7
31	Ga	69	690.94	0.02	1.18E-02	1.4
31	Ga	71	834.03	0.03	7.52E-02	3.1
32	Ge	70	499.97	0.02	9.57E-03	2.4
32	Ge	72	297.42	0.03	2.51E-03	5
32	Ge	73	595.88	0.02	6.91E-02	3.0
32	Ge	74	253.22	0.03	3.68E-03	5
33	As	75	165.09	0.03	4.03E-02	3.0
34	Se	76	6600.67	0.12	2.31E-02	4.7
34	Se	77	1308.60	0.04	1.44E-02	4.6
35	Br	79	1249.69	0.02	2.07E-03	2.3

Z	El	A	E keV	unc. keV	k_0(H)	unc. %
35	Br	81	287.76	0.03	9.60E-03	5
37	Rb	85	556.81	0.03	3.24E-03	2.7
37	Rb	87	196.34	0.03	3.42E-04	5
38	Sr	86	388.53	0.02	1.79E-03	5
38	Sr	87	1836.05	0.03	3.53E-02	1.3
39	Y	89	6080.12	0.07	2.90E-02	1.8
40	Zr	91	934.47	0.06	4.15E-03	3.0
41	Nb	93	499.49	0.03	2.12E-03	7
42	Mo	95	778.22	0.01	6.43E-02	2.3
42	Mo	97	787.40	0.02	5.38E-03	3.2
44	Ru	99	686.89	0.01	4.59E-02	9
45	Rh	103	470.41	0.03	7.37E-02	2.6
46	Pd	105	616.22	0.02	1.82E-01	1.0
46	Pd	108	433.60	0.03	2.96E-03	1.6
47	Ag	107	657.74	0.02	5.42E-02	2.2
48	Cd	113*	558.32	0.03	5.03E+01	1.6
49	In	115	5892.38	0.15	5.65E-02	10
50	Sn	115	1293.53	0.06	3.42E-03	1.6
50	Sn	117	1229.64	0.06	1.72E-03	1.9
50	Sn	120	925.90	0.06	2.49E-04	3.0
51	Sb	121	921.04	0.04	8.55E-02	4.2
51	Sb	121	6523.9	0.2	8.33E-02	5
51	Sb	123	598.66	0.05	1.53E-02	3.7
52	Te	123	602.72	0.01	5.63E-02	10
53	I	127	898.58	0.07	3.71E-02	10
54	Xe	124	600.22	0.09	1.25E-02	20
54	Xe	128	586.23	0.10	1.12E-02	20
54	Xe	129	536.29	0.09	3.94E-02	20
54	Xe	131	667.87	0.09	1.59E-01	20
55	Cs	133	5505.5	0.2	6.98E-03	5
56	Ba	135	818.47	0.05	4.68E-03	2.1
56	Ba	136	1898.47	0.08	6.29E-04	3.7
56	Ba	137	1435.65	0.06	6.80E-03	2.6
56	Ba	138	627.31	0.05	6.47E-03	2.1
57	La	139	567.41	0.02	7.27E-03	2.9
58	Ce	136	712.25	0.06	2.61E-04	8
58	Ce	140	662.03	0.05	5.04E-03	8
58	Ce	142	1186.75	0.06	1.44E-03	8
59	Pr	141	176.95	0.03	2.45E-02	5
60	Nd	142	742.09	0.02	6.65E-02	2.6
60	Nd	143	696.49	0.02	7.20E-01	5
60	Nd	145	453.92	0.02	6.57E-02	2.9
62	Sm	149*	334.03	0.05	9.65E+01	1.3
62	Sm	149*	737.49	0.05	1.21E+01	1.3
63	Eu	151*	89.97	0.08	2.85E+01	1.8
63	Eu	151*	841.59	0.01	5.46E+00	3.1
64	Gd	155*	79.71	0.06	7.78E+01	2.6
64	Gd	157*	1186.75	0.05	6.07E+01	6
65	Tb	159	63.74	0.08	2.78E-02	11
65	Tb	159	74.89	0.08	3.39E-02	10
66	Dy	161	185.19	0.09	5.10E-01	2.6
66	Dy	163	415.03	0.07	4.64E-01	2.8
66	Dy	164	184.34	0.07	2.21E+00	10
67	Ho	165	116.84	0.04	1.49E-01	5
67	Ho	165	136.67	0.04	2.66E-01	5
68	Er	166	207.82	0.03	3.89E-02	3.7
68	Er	167	184.30	0.03	1.01E+00	9
69	Tm	169	149.66	0.05	1.28E-01	1.7
69	Tm	169	204.41	0.05	1.56E-01	2.1
70	Yb	168	812.69	0.04	1.99E-02	10
70	Yb	171	3942.8	0.4	6.44E-03	10
70	Yb	173	363.33	0.03	1.57E-02	10
70	Yb	174	514.87	0.03	1.58E-01	10
70	Yb	176	3644.8	0.4	5.41E-03	11
71	Lu	175	71.46	0.07	6.85E-02	3.9
71	Lu	175	192.00	0.06	3.62E-02	3.9
72	Hf	177	325.55	0.06	7.98E-02	4.0
72	Hf	178	5723.9	0.15	3.35E-02	2.4
73	Ta	181	270.48	0.06	4.36E+02	1.6
74	W	182	5164.24	0.15	5.52E-03	3.8
74	W	183	6190.6	0.2	1.25E-02	3.5
75	Re	187	207.92	0.04	7.36E-02	5
76	Os	190	5146.63	0.15	6.51E-03	4.8
77	Ir	193	5667.8	0.2	3.82E-02	7.4
78	Pt	195	355.54	0.04	9.77E-02	0.9
78	Pt	196	5097.6	0.2	1.47E-03	7
79	Au	197	215.01	0.03	1.21E-01	1.5
79	Au	198	411.80	0.02	1.46E+00	1.5
80	Hg	199	367.96	0.03	8.02E-01	4
81	Tl	203	873.16	0.08	2.49E-03	3.8
82	Pb	204	6729.27	0.13	4.67E-05	3.1
82	Pb	207	7367.83	0.12	2.00E-03	2.4
83	Bi	209	4170.96	0.11	2.45E-04	13
90	Th	232	583.27	0.09	3.64E-03	10
92	U	235	6395.16	0.15	4.05E-05	13
92	U	238	4060.34	0.04	2.36E-03	1.3

* Non-1/v nuclide

d) From $^{10}B(n,\alpha\ \gamma)^{7}Li$ reaction, uncertainty is the approximate peak width.
e)-i) Decay γ rays

Table 2. Sample page from the new Catalogue

Z	Element symbol	E_γ (keV)	*±SD (keV)*	$\theta \cdot I_\gamma \cdot \sigma$ (b)	*±RSD (%)*	Relative intensity	E_γ/ENSDF (keV)	Isotope A	Comment
1	H	2223.26	*0.02*	3.33E-01	*0.2*	100.0	2223.225	1	
1	D	6250.20	*0.10*	4.92E-04	*5.0*	100.0	6250.140	2	100% D
3	Li	477.59	*0.05*	1.40E-03	*5.9*	3.5	477.590	6	
3	Li	980.56	*0.05*	4.36E-03	*5.1*	11.0	980.600	7	
3	Li	1051.82	*0.05*	4.36E-03	*5.1*	11.0	1052.000	7	
3	Li	2032.31	*0.07*	3.98E-02	*5.0*	100.0	2032.500	7	
3	Li	6769.63	*0.26*	1.35E-03	*6.5*	3.4	6768.780	6	
3	Li	7246.80	*0.28*	2.11E-03	*8.4*	5.3	7245.870	6	
4	Be	219.39	*0.10*	4.71E-06	*17.7*	0.1	219.300	9	
4	Be	547.58	*0.04*	1.02E-05	*10.1*	0.2	547.400	9	
4	Be	631.92	*0.04*	1.12E-05	*10.0*	0.2	631.800	9	
4	Be	853.63	*0.01*	1.65E-03	*8.9*	26.7	853.500	9	
4	Be	2590.01	*0.03*	1.88E-03	*8.9*	30.4	2590.200	9	
4	Be	2811.66	*0.16*	1.04E-05	*13.2*	0.2	2811.800	9	
4	Be	2896.17	*0.11*	1.13E-05	*12.3*	0.2	2896.400	9	
4	Be	3367.48	*0.04*	2.92E-03	*8.9*	47.3	3367.600	9	
4	Be	3443.42	*0.04*	9.93E-04	*8.9*	16.1	3443.500	9	
4	Be	5956.60	*0.09*	1.46E-04	*9.1*	2.4	5956.700	9	
4	Be	6809.58	*0.10*	6.18E-03	*9.0*	100.0	6809.400	9	
5	B	477.60	*5.00*	7.13E+02	*0.3*	100.0	477.590	10	(n,αγ)

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Evaluation and measurement of prompt k_0 -factors to use in prompt gamma-ray neutron activation analysis

As a prt of
CO-ORDINATED RESEARCH PROJECT:
Development of a Data base for Prompt Gamma-ray Neutron Activation Analysis

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PROJECT REPORT

Prompt gamma-ray neutron activation analysis (PGNAA) is a complementary technique to conventional neutron activation analysis (NAA) method and is capable of analysing elements like H, B, C, N, P, S, Si, Cd, Gd, Sm and Eu. In PGNAA prompt γ-rays are measured following neutron capture reaction. Since on-line measurements of characteristic prompt gamma-rays from the sample are involved, good shielding for both the sample and detector for neutron and γ-rays is required. The prompt γ-rays are assayed by high purity germanium detector (HPGe) coupled to a PC-based multi channel analyser (MCA). Neutrons from a thermal or cold neutron guided beam are used for PGNAA system.

In the case of k_0 -method in PGNAA one has to determine the prompt k_0-factors for the elements. A k_0 -factor for the element x to the comparator c is given as:

$$k_{0,c}(x) = \frac{(A_{sp}/\varepsilon)_x}{(A_{sp}/\varepsilon)_c} = \frac{M_c\theta_x\sigma_x\gamma_x}{M_x\theta_c\sigma_c\gamma_c}$$

$$k_0(\text{exp}erimental) = \frac{(A_{sp}/\varepsilon)_x}{(A_{sp}/\varepsilon)_c} \;\; and \qquad k_0(theoretical) = \frac{M_c\theta_x\sigma_x\gamma_x}{M_x\theta_c\sigma_c\gamma_c}$$

where, A_{sp} = count rate per unit weight of the element i.e., elemental sensitivity, M = atomic mass, θ = isotopic abundance, σ = thermal neutron capture cross section, γ = prompt gamma-ray abundance, ε = absolute full-energy peak detection efficiency.

Determination of experimental k_0-factors are important due to uncertainties on absolute values of σ and γ. Determination of absolute full-energy peak detection efficiency and elemental sensitivity are required to obtain experimental k_0-factor.

PGNAA SYSTEM:

Work has been initiated to install a PGNAA system in 100 MW Dhruva reactor facility in BARC, Trombay, Mumbai, India. A thermal guided beam facility is available in this reactor where the neutron beam is transported through the beam tube to about 30 meters away from the reactor core. An experimental set up has been arranged for PGNAA using this guided beam. The dimension of the beam is 2.5 cm x 10 cm. The shielding materials used at present are boron carbide for avoiding scattered neutrons towards the detector followed by 30 cm thick lead bricks for reducing gamma-ray background. The γ-ray detector is located at about 40 cm distance from the sample and is placed at 90^0 with respect to the beam direction. A collimator is used in front of the detector to collimate the gamma-rays coming from the sample.

Experimental:

Neutron beam calibration:

Effective neutron flux at sample irradiation position has been determined using gold as flux monitor. Known amount of gold was irradiated and off-line counting of irradiated sample was carried out using a 15% HPGe detector coupled to a 4k channel analyser. The measured neutron flux is about $2\text{x}10^7$ $n.cm^{-2}.s^{-1}$. Cadmium ratio method was used to ascertain the thermal component of the flux. No activity could be detected in the irradiated gold sample wrapped with 0.8 mm thick cadmium foil. Using indium foil as flux monitor, cadmium ratio was found to be $1.7\text{x}10^3$ indicating negligible epithermal component.

Detection system:

A 22% HPGe detector connected to a PC based 8k MCA has been used for counting prompt gamma-rays. The resolution of the detector is 2.4 keV at 1332 keV. The MCA has been calibrated in the region of 0.1 to 9 MeV using the delayed gamma-rays from ^{152}Eu and ^{60}Co and prompt gamma-rays from ^{36}Cl. A second order polynomial is used for the energy calibration.

Prompt gamma-ray spectra:

Samples weighing in the range of 100-300 mg were wrapped in thin Teflon (polytetrafluroethylene-PTFE) ribbon. Prompt gamma-ray spectra of different elements were collected exposing the suitable compounds of the elements to the beam for 1 to 24 hours to identify their characteristic gamma lines. For example, gamma-ray spectra of elements from samples like NH_4Cl, NaCl, KCl, $HgCl_2$ and Ti metal were collected. The capture gamma-ray table by Lone et al. was followed for identifying the prompt gamma-ray lines of different elements.

Efficiency calibration:

The delayed gamma-ray from ^{152}Eu and prompt gamma-ray from ^{36}Cl were used for detection efficiency calibration. Ammonium chloride salt, packed in Teflon, was irradiated for about 24 hours and the capture gamma-rays were accumulated. The data on absolute gamma-ray intensities for the above isotopes were taken from IAEA-TECDOC-619. The ^{36}Cl serves as efficiency standard for a wide range of energies i.e., 0.5 to 8.5 MeV. The absolute full energy peak efficiencies were determined for low energy region (i.e., upto 1500 keV) using ^{152}Eu source and the relative efficiency plot for the energy region from 0.5 to 9 MeV was obtained from the prompt gamma-ray spectrum of ^{36}Cl. The relative efficiencies obtained from the chlorine spectrum was normalised to ^{152}Eu efficiencies to obatin absolute detection efficiencies of the gamma-rays. The typical efficiency values are in the order of 10^{-4} to 10^{-5}. The energy vs. efficiency curve is shown in Fig.1.

The k_0 determination:

Due to uncertainties on gamma-ray intensities and capture cross section for a particular isotope the theoretical k_0-factor can not be used as input parameter in the case of PGNAA. The k_0-factor is being determined for lighter elements with respect to 1951 keV line of ^{36}Cl using the elemental sensitivity and the respective efficiencies of the gamma lines. The experimental determination k_0 for the elements like H, Na, K, Ca, and Hg are in progress.

Future Work Plan:

1. Improved shielding arrangements both for neutron and gamma-rays.
2. Use of Compton suppressed spectrometer system.
3. Determination of k_0 factors for lighter elements.
4. Updating of the data based on the information published since 1980.
5. Determination of absolute capture gamma-ray intensities of some of the isotopes.

Acknowledgement: We are thankful to the Head, Condensed Matter Physics Division, BARC for providing the guided thermal neutron beam facility for our experiments.

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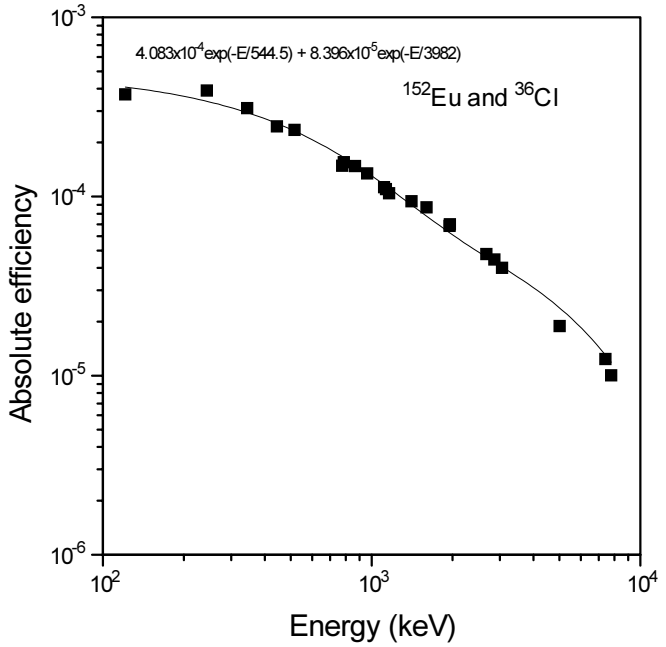

Fig.1: Absolute efficiency vs. Energy of Gamma-ray

MEASUREMENT OF Ko-FACTORS FOR SOME ELEMENTS IN PROMPT GAMMA NEUTRON ACTIVATION ANALYSIS

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INTRODUCTION

The Dalat nuclear research reactor has been operated since February 1984 after completing the reconstruction and upgrade of the old one. In 1989 the tangential beam port of the reactor has been used for the prompt gamma neutron activation analysis (PGNAA). Recently, the PGNAA has been developed for in-vivo determination of some toxic elements in organs such as kidney and liver using the filtered fast neutron beam of 144 keV at the radical beam port. In the framework of the IAEA Research Contract No.10734 "*Measurement of Ko-factors for some elements in prompt gamma neutron activation analysis*", the standardization and characterisation of the PGNAA facility including the thermal neutron beam and the spectrometer at the Dalat reactor for this purpose have been conducted. The report presents a review of the status of neutron beam utilization at the reactor and some recent results obtained in the framework of the Research Contract such as upgrade of beam quality, detection efficiency of the spectrometer, and the future plan.

DALAT NUCLEAR RESEARCH REACTOR

The Dalat Nuclear Research Reactor (DNRR) is a pool type research reactor which was reconstructed in 1982 from the previous 250 kW TRIGA MARK II reactor installed in 1963. The reconstruction had been completed in the end of 1983. The reactor core, the control and instrumentation system, the primary and secondary cooling systems as well as other associated systems were newly designed and installed. The core is loaded with VVR-M2 fuel elements with 36% enrichment. The renovated reactor reached its initial criticality in November 1983 and attained its nominal power of 500 kW in February 1984. The main characterictis of the reactor are given in Table 1. The maximum thermal neutron flux is 2.1×10^{13} n/cm^2/s. Since the DNRR has been operated with the contineuosly working schedule of 100 hours for every 4 weeks and used mainly for research, isotope production, neutron activation analysis and training. The such working schedule of the reactor has limited many aplications where long time irradiation is requested.

Table 1: *Main characteristics of the Dalat reactor*

Parameter	Value
Power, kW	500
Fuel	U-Al alloy
Number of fuel bundles in the core	100
Enrichment, %U-235	36
Moderator and coolant	Light water
Core cooling mechanism	Natural convection
Effective delayed-neutron fraction, %	0.81
Current excess reactivity, $	6.5
Temperature and power effects, $	-0.36
Equilibrium xenon poisoning, $	-1.69
Control rod worth, $:	
- Shim rod No.1	2.97
- Shim rod No.2	3.09
- Shim rod No.3	2.70
- Shim rod No.4	2.50
- Regulating rod	0.5
- Two safety rods	5.36
Thermal neutron flux at 500 kW power ($n/cm^2/s$):	
- Neutron trap	2.1×10^{13} (R_{Cd}=3.2)
- Channel 7-1 (wet)	5.1×10^{12} (R_{Cd}=2.5)
- Channel 13-2 (dry)	4.2×10^{12} (R_{Cd}=2.3)
- Rotary specimen rack	3.2×10^{12} (R_{Cd}=6)
- Center of the thermal colunm	4.5×10^{10} (R_{Cd}=54)
- Horizontal beam tube No.1	2.0×10^{12} (R_{Cd}=4.3)
	1.5×10^{10} (E>3MeV, S-foil activation)
- Horizontal beam tube No.2	9.0×10^{11} (R_{Cd}=6.6)
	7.5×10^{9} (E>3MeV, S-foil activation)
- Horizontal beam tube No.3	1.2×10^{12} (R_{Cd}=3.6)
	2.9×10^{10} (E>3MeV, S-foil activation)
- Horizontal beam tube No.4	5.0×10^{12} (R_{Cd}=4.3)
	5.7×10^{11} (E>3MeV, S-foil activation)
Maximum surface temperature of fuel	97.2 ^{o}C
Maximum water temperature of the core	54.5 ^{o}C

NEUTRON BEAM UTILIZATION

Neutron beam utilization is one of the main activities of DNRR. So far, this activity has been focused on development of filtered neutron beams and performance of research and applications using these filtered neutron beams. Review of this activity is given in /1,2,3/. Summary of this activity is as following:

1. Creation of filtered neutron beams at 144 keV, 75 keV, 55 keV, 25 keV as well as thermal neutron beam using the filtered technique.
2. Measurement of total neutron cross sections on these filtered beams using the transmission method.

3. Measurement of avarage radiative capture cross sections by the activation method.
4. Set up experiments for research on average resonance capture in collaboration with the Kiev Institute for Nuclear Research (Ukraine). However, due to the financial limitation, the work is not in progress.
5. Performance of research on (n,2γ) reaction using the method of the summation of amplitudes of coincident pulses (SACP) is carrying out.
6. Development and performance of research on neutron radiography using the thermal neutron beam at the tangential port of the reactor.
7. Development and application of the prompt gamma neutron activation analysis using the thermal neutron beam at the tangential port of the reactor.
8. Development and performance of research on the in-vivo PGNAA using the fitered neutron beam at 144 keV at the radical port of the reactor.

PROMPT GAMMA NEUTRON ACTIVATION ANALYSIS

The gamma background in prompt-gamma measurements has been investigated by using cellulose samples which were irradiated as in the PGNAA experiment.

The effect of neutron self-shielding and gamma self-absorption has been investigated. The results showed that with the increase of the sample weight from 0.5 to 5 gram, the influence of the effect was not recognized.

The analytical sensitivities of recommended gamma lines which are the most sensitive were obtained by the irradiation of pure elements or compounds in the form of foil or pellet. On the basis of these sensitivities, K-factors representing sensitivity ratios relative to K, Si, Cl were calculated. Table 2 shows the sensitivities and K-factors of some elements obtained by ourselves.

In order to verify the reliability of our PGNAA system, analysis of Standard Reference Materials such as IAEA-SL-1, Pond Sediment NIES has been carried out. A good agreement with the certified or reference values is seen in Table 3. The prompt gamma spectrum of the IAEA-SL-1 is shown in Fig 1.

Our PGNAA system has been used for analyzing a variety of samples such as biological, geological, environmental samples, for example:

- Determination of boron in several reference materials (See Table 4). It is seen that boron in a content range larger than 10 ppm can be analyzed in a variety of samples with satisfactory accuracy. For the content of boron lower than 10 ppm, there was discrepancy in our analytical results. So, at the ppm level, the correction for boron background can affect the accuracy and precision of analysis and needs to be further investigated.

- Determination of major and minor elements in some environmental samples (See Table 5: The concentration of Al, Fe, Ti, Si, Ca, K in airborn dust samples which were collected monthly at Hochiminh city).

- Etc.

Table 2. The sensitivities and K-factors obtained by PGNAA at the Dalat reactor

Element	E_γ (KeV)	Sensitivity (c/g/s)	K-factor(%) K_{Si}(3539 KeV)	K-factor(%) K_{Cl}(788 KeV)	K-factor(%) K_K(771 KeV)
H	2223	5.61	95.3(3)	1.399(2)	13.4(2)
C	4945	0.002	0.037(7)	0.00055(10)	0.0052(8)
N	1884	0.021	0.356(5)	0.0052(8)	0.050(6)
Al	1778	0.244	4.14(4)	0.061(6)	0.581(5)
Si	3539	0.059	1.0	0.0147(4)	0.140(4)
P	3900	0.016	0.271(7)	0.004(8)	0.038(6)
S	2380	0.11	1.86(6)	0.0275(8)	0.2619(5)
Cl	788	4.01	67.9(4)	1.0	9.55(2)
K	771	0.42	7.12(4)	0.1047(2)	1.0
Ca	1943	0.112	1.90(5)	0.028(3)	0.267(4)
Ti	342	0.082	1.39(4)	0.0204(3)	0.195(3)
Mn	847	0.861	14.6(5)	0.215(3)	2.05(4)
Fe	1725	0.112	1.90(6)	0.028(6)	0.267(6)

Table 3. Analytical results of IAEA-SL-1 and NIES-CRM-2 by PGNAA

	Lake Sediment IAEA-SL-1		Pond Sediment NIES-CRM-2	
Element	This work	Reference	This work	Reference
B (ppm)	36 ± 3	39 (N)	32.5 ± 3	
Ti	4734 ± 211	5170 ± 327	6897 ± 233	6400 (N)
Mn	3367 ± 181	3460 ± 159	748 ± 48	770 (N)
Ca	2105 ± 321	2500 (N)	7195 ± 1942	8100 ± 599
Si (%)	27.6 ± 0.3		21.3 ± 0.2	21.0 (N)
Fe	6.87 ± 0.45	6.74 ± 0.17	6.68 ± 0.51	6.53 ± 0.35
Al	8.5 ± 0.7	8.9 (N)	11.3 ± 0.9	10.6 ± 0.5
K	1.22 ± 0.07	1.50 (N)	0.71 ± 0.05	0.68 ± 0.06

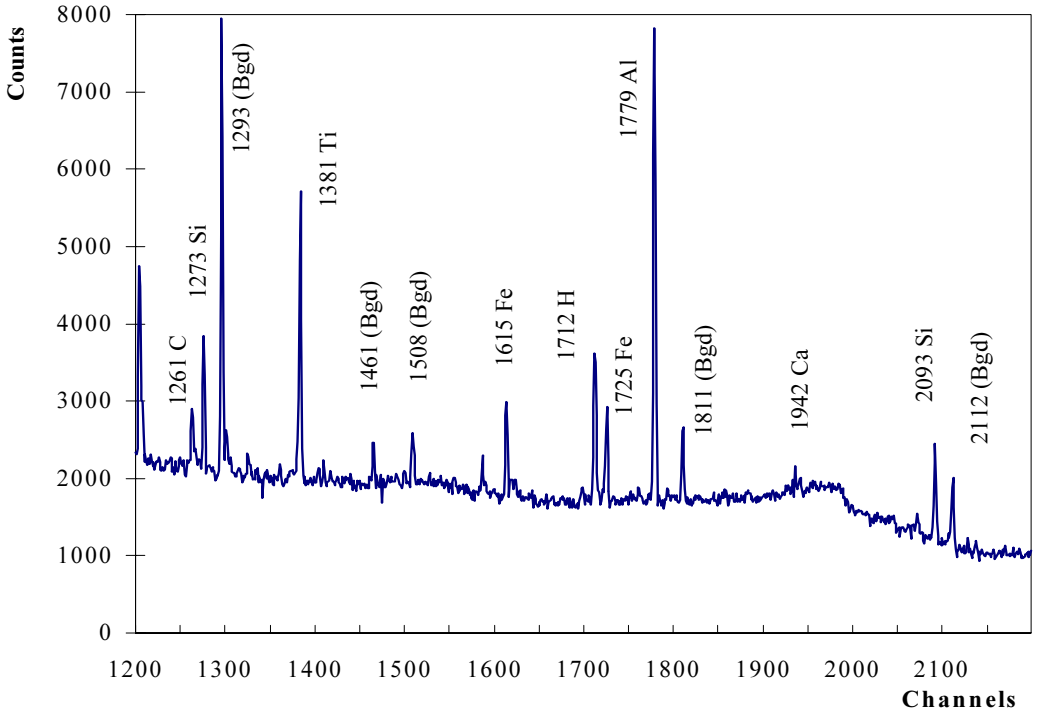

Fig 1. A portion of the prompt gamma spectra of the SL-1 sample

Table 4. The results of the determination of B in some Reference Materials.

Samples	This work	Other work	Cert.*
SRM 1572 Citrus	69.7 ± 4.5	63.5 ± 1.3	
Leaves	34.2 ± 3.5	38.3 ± 0.8	30
SRM 1573 Tomato	32.4 ± 4	28.1 ± 0.7	30
SRM 1570 Spinach	30.1 ± 3.5	32.0 ± 0.6	33.3 ± 3
SRM 1571 Orchard	19.3 ± 2	17.1 ± 0.4	
Leaves	3.1 ± 1.2	1.72 ± 0.21	
SRM 1575 Pine	2.1 ± 0.8	0.40 ± 0.19	
Needles	3.1 ± 1.1	2.52 ± 0.25	1.7
SRM 1549 Milk Powder	54.6 ± 6	51.1 ± 0.3	49 ± 6
SRM 1577 Bovine Liver			
IAEA -A-11 Milk Powder			
Bowens Kale			

* Information values if uncertainty is not given

Table 5. Analytical results of aerial dust samples in Hochominh city

Element	Dust-12		Dust-13		Dust-14	
	PGNAA	Others	PGNAA	Others	PGNAA	Others
Fe (%)	2.98 ± 0.47		3.94 ± 0.4	3.6	4.56 ± 0.38	4.3
Al (%)	3.2		3.32 ± 0.21	3.0	5.45 ± 0.70	4.8
K (%)	2.37 ± 0.33		1.34 ± 0.14	1.15	0.91 ± 0.08	1.05

Ca (%)	2.3		7.81 ± 0.69	8.6	5.87 ± 0.45	5.4
Ti(%)	1.17 ± 0.09		0.39 ± 0.04	0.42	0.39 ± 0.05	0.36
Si (%)	1.4		22.36 ± 1.99	20.3	15.23 ± 1.12	17.4
	6.13 ± 0.58					
	5.7					
	0.30 ± 0.04					
	0.28					
	18.47 ± 1.21					
	17.0					

UPGRADE THE PGNAA FACILITY FOR Ko-FACTOR MEASUREMENT

In the relative analytical method, the beam quality and the detection efficiency curve of the spectrometer are not needed to be known exactly. However, for the Ko-factor measurements, they must be known as exactly as possible.

We have made the reconstruction of shieldings for our spectrometer, collimators for neutron beam and suitable neutron filters arrangement in order to receive a good quality of the neutron beam, low gamma background and reduction of radiation damage for the spectrometer. Fig.2 and 3 show the sectional view of the lay-out of the shield and arrangement of the spectrometer, and the sectional view of the tangential beam tube No.3 of the Dalat reactor.

In order to receive the thermal neutron beam with a good quality for Ko-factor measurements, we have used different combinations of filters from lead, graphite and monocrystal silicon. As shown in /4/, the silicon monocrystal filters allow to receive a good thermal neutron beam from the tangential tube of reactor with very low neutron background of high energies. At our current condition, we could not measure the spectrum of the thermal neutron beam. So we can only evaluate the quality of the thermal neutron beam by two parameters as the absolute thermal neutron flux and the cadmium ratio. The activation method has been used for this purpose. Activation Au-foils and cadmium covers made in USA (Reactor Experiments INC, Belmont, California) has been used in our experiments. Table 6 shows dependence of thermal neutron beam characteristics on filters combinations. The 8 cm graphit and 5 cm lead had been fixed at the inside of the beam tube when we contructed the neutron beam (See Fig.3). The second part of the beam tube where neutron filters are put into can be changed. In this experiment we used only silicon monocrystal filters. It can be seen that the neutron flux decreases not so much along with the increase of silicon length, however, the cadmium ratio increases significantly. So we expect to use as much silicon lengths as we have.

Table 6: The variation of neutron flux and cadmium ratio with silicon filters lengths

Filters combinations	Neutron flux ($n/cm^2/s$)	Cadmium ratio
8 cm C + 5 cm Pb + 50.0 cm Si	4.83×10^6	224.6
8 cm C + 5 cm Pb + 52.8 cm Si	4.09×10^6	268.7
8 cm C + 5 cm Pb + 55.8 cm Si	3.65×10^6	290.7
8 cm C + 5 cm Pb + 60.3 cm Si	2.78×10^6	409.3
8 cm C + 5 cm Pb + 66.3 cm Si	2.67×10^6	524.0

8 cm C + 5 cm Pb + 71.0 cm Si	2.44 x 10^6	775.6

To determine the Ko-factors according to the principle of the Ko-standardization approach /5/, we must know the relative efficiency curve of the spectrometer in the PGNAA experiment. In the low energy region, we have used the activated Eu-sample with the same geometry as that of samples which will be used later on in Ko-factor measurements. In the high energy region we have used the prompt gamma rays from Cl. The efficiency curve of the spectrometer was contrusted by least-squares fitting to a polynomial with a precision of 1-2% in the energy range (E<5000 keV) and 3-5% in the energy range (E>5000 keV) as shown in Fig.4. This efficiency curve will be used to determine Ko-factors with taking into account the uncertainty of the fitted efficiency curve.

WORKING PLAN FOR THE NEXT TIME

- To choose a suitable length of silicon filters in combination with other filters with the aim of getting as good quality of the thermal neutron beam as possible. Determine characteristics of the beam such as neutron flux, cadmium ratio and gamma dose rate.
- To improve a precision of the efficiency curve of the spectrometer.
- Measurement of Ko-factors instoichiometric compounds related to the 1951 keV gamma ray of Cl for the elements as C, Na, K, Cr, Mn, Fe, Co, Ni, cu, cd, Ba, Ti, sm, Gd, Hg, Pb, etc.
- Make the date available to the IAEA/NDS.
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A User's Perspective on Data Quality and Accessibility

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The history of neutron-capture prompt gamma-ray activation analysis (PGAA) at the NIST reactor began in 1977 with a project headed by Professors Glen Gordon, William Walters, and William Zoller at the University of Maryland. The hard work was done by Michael Failey as a PhD student, and by David Anderson, first as a postdoctoral fellow at Maryland and up to the present as a staff member of the US Food and Drug Administration. We built a PGAA system around a well-collimated, unfiltered, vertical thermal-neutron beam and a large (for its time) Ge gamma detector. The 20-MW heavy-water NBSR operates continuously for 38-day fuel cycles to produce a thermal neutron PGAA beam 3.5 cm in diameter with fluence rate $3x10^8$ n/cm^{2}s. The same system (although the detector has been replaced at least once and the MCA is in its third generation) is still in almost constant analytical use, the log book listing over 12,000 spectra. Only a 53 mm thick sapphire filter has been added to the original system; the external components are now under more comprehensive redesign.

At the beginning of this project there were few available data tables useful for interpreting Ge spectrometer data [1-7]. The only comprehensive measurements of the capture gamma rays of the elements were Rasmussenís at MIT, available only as technical reports. Duffeyís compilations, the first publication in the open literature of those measurements, tabulated some of those data from the userís point of view, including sensitivity factors $I\sigma/A$ and spectral contrast (strong or weak) for each gamma ray.

Beginning from these resources, for analytical purposes the Maryland group (with concurrent developments by Gladney, Curtis, and Jurney at Los Alamos and by Glascock at Missouri) found it necessary to work out the identity of escape peaks and interferences. The Maryland group used a split-annulus scintillator as a Compton - pair spectrometer, accumulating three spectra from at least two sources of material for each element. Our first publication [8] included a table of recommended lines for 22 elements and their principal interferences.

Loneís 1981 publication of the Rasmussen data [9] was a great step forward: a large compendium with 10,200 lines. It is remarkable how useful this paper, based on measurements in the early days of Ge detectors, has retained its value. We still use the Lone table, both in print and a subset in spreadsheet form (1042 lines, from the diskette in ref. 10), as our first resource for identification. Copies in both forms are kept at hand near the PGAA spectrometer console. This useful compilation has, however, three serious flaws:

1. Data for many elements are incomplete. The arbitrary low-energy cutoff of 200 keV (sometimes 300 keV) eliminates the strongest lines of Ga and Gd, for example. Not all the capture energy is accounted for.

2. Analytically useful lines which do not result from (n,γ) reactions are omitted. The most prominent example is the boron line at 478 keV from the (n, α) reaction, but short-lived activation products, prominent in the irradiation of many materials, are also missing.

3. Many peaks are misidentified. The lines listed for Ce at 335, 440, and 738 keV are probably due to a Sm impurity. Thirty-eight elements have a line listed near 559 keV, probably many of them from Cd neutron shielding in and near the apparatus.

Accessibility

Of course a great deal of work has been done since Rasmussen on the careful evaluation of level schemes populated by neutron capture, but the most accessible source of data is still the paper by Lone et al. Because it was constructed by and for nuclear structure physicists, the ENSDF database is not readily accessible to chemists.

Printed copies of data are still needed, supplemented by tabular data in computer-readable form. Both are needed, as an example from my own experience shows: Appendix 1 (atomic weights and other elemental properties) of the BNL Nuclear Wallet Cards is available as a PDF or PostScript file, but not (except by special request) as a table. I asked the fine people at BNL, copied the table to my Macintosh with ftp, edited out the spaces with Word Perfect, and read it into an Excel spreadsheet for use in calculating radioactivity from neutron irradiations. This procedure gave me the best evaluated data for my calculations, but was so cumbersome that I have made mistakes in editing, which may not all have been corrected yet.

The Lone table was compact and readable, only 89 pages (compared with 716 pages by Bartholomew, Groschev, et al.). It should not be too much to expect that *Atomic and Nuclear Data Tables* will print a new compilation of comparable size.

It is an open question whether Web pages are citeable as references in the professional literature. Certainly they are not peer reviewed in the conventional sense, however definitive they may be. Web pages are ephemeral: if you follow random links on the Web, some will have disappeared except for the smile.

New developments

We have been performing PGAA with cold neutrons since 1986, experimentally at KFA J¸lich in 1986 [11], and then with our own instrument at NIST since 1990 [12,13]. Cold neutrons bring several benefits:
Greater sensitivity (higher flux, larger cross section)
Simpler shielding and collimation
Better background, especially for hydrogen

But thermalization (warming) of cold neutrons in non-thin samples changes the reaction rate and therefore brings problems in quantitation. In large part, the use of ratios of reaction rates to an internal standard solves this and other problems [14, 15].
A particular case of element ratios in activation analysis is called the k_0 method. Applied to cold-neutron PGAA this approach is particularly simple [16].
The defining equation is

where

A = counting rate at energy $E\gamma_g$
m = mass of element
θ = abundance of the capturing isotope
Γ = gamma yield in photons per capture
M = atomic weight
σ = capture cross section
εe = counting efficiency

The subscripts x and s refer to the element of interest and the reference element, respectively. Cold- and thermal-neutron values relative to titanium, chlorine, and hydrogen have been measured at NIST, and more completely at Budapest [17].

Conclusion

In his 1981 critical review of the Lone manuscript, Professor Gordon said ìItís probably going to be necessary to re-run Rasmussenís experiments with a highly calibrated, computer-based spectrometer and operators that know about impurities and other artifacts.î Nearly twenty years later, we finally have such a remeasurement of all elements at Budapest. I look forward eagerly to its publication, and even more to the integration of these new data with the ENSDF database that is the subject of this CRP.

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Interactive Visual Analysis of Remote/Local Nuclear Data

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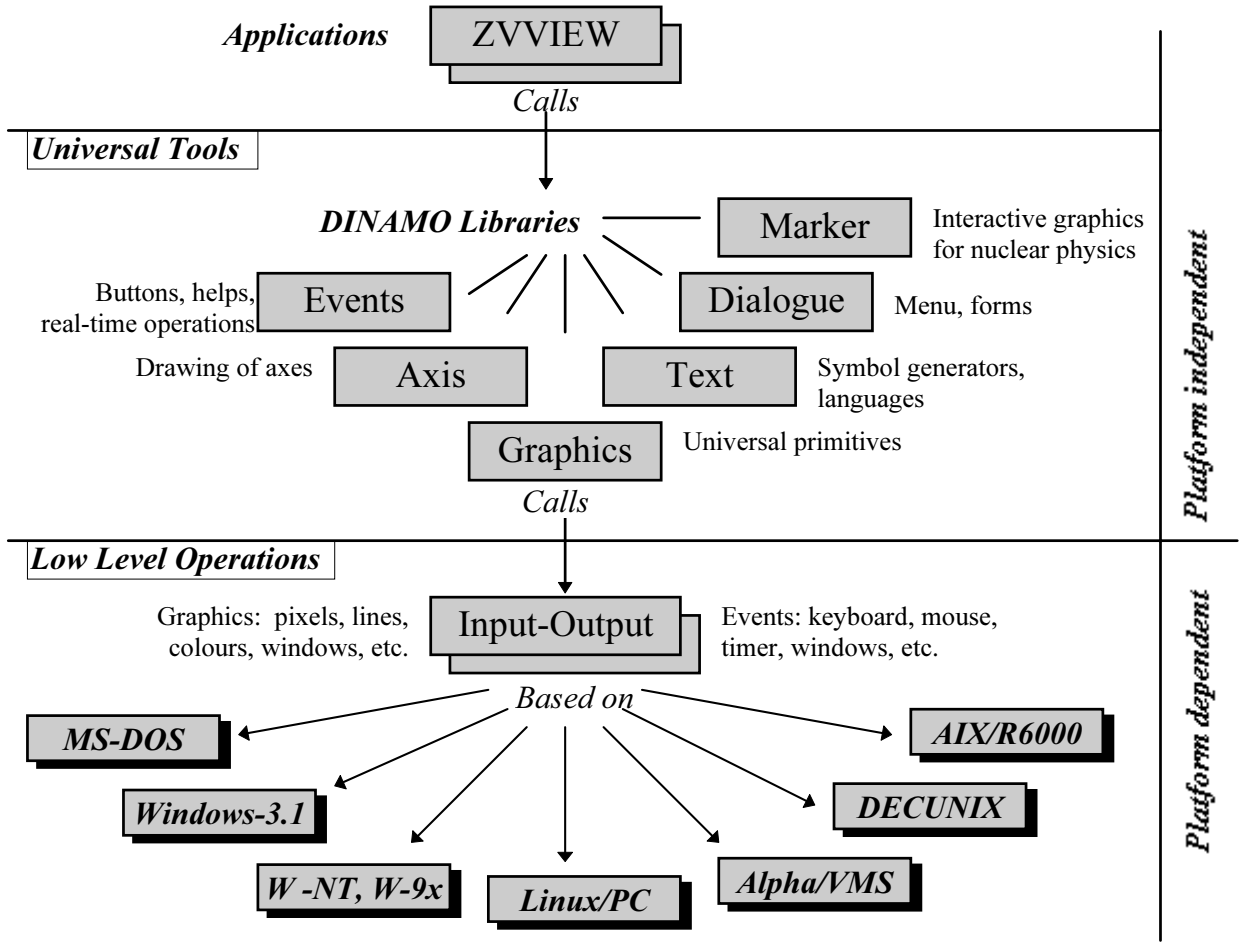
ZVView is a software designed for nuclear reactions data evaluators to perform efficient interactive visual analysis of cross section data retrieved from EXFOR and ENDF libraries. The main function of ZVView is plotting and inter comparison of data, including variety of options for looking into numerous details of graphical, numerical and bibliographic information involved, along with a possibility to analyse results of own evaluation. ZVView allows to user change of plotting attributes, logarithmic and linear scales, zooming, split plot to sub-windows, smoothing by least square method, choice and authors to be plotted and scan their points, changing language on the fly, saving picture in Postscript and PCX formats, etc. And this all on many computer platforms.

ZVView is written on C and based on DINAMO, a universal graphic set (package) of libraries. Originally, this package was developed to be common basic software for development of various applications for nuclear research, such as acquisition, data treatment, analysis and presentation. The main functions of package are related to plot on the screen, compare and analyse in interactive way functions of the type *f(x)* and *f(x,y)*. Variety of application fields, tasks, requests from number of users during several years of using, caused flexible structure of the package, universality related to data structures, rich and expandable functionality, fast speed of operations and small memory needed. One of the most attractive feature of the package is that it works on several computer platform, therefore, an application (such as ZVView) based on DINAMO are platform independent.

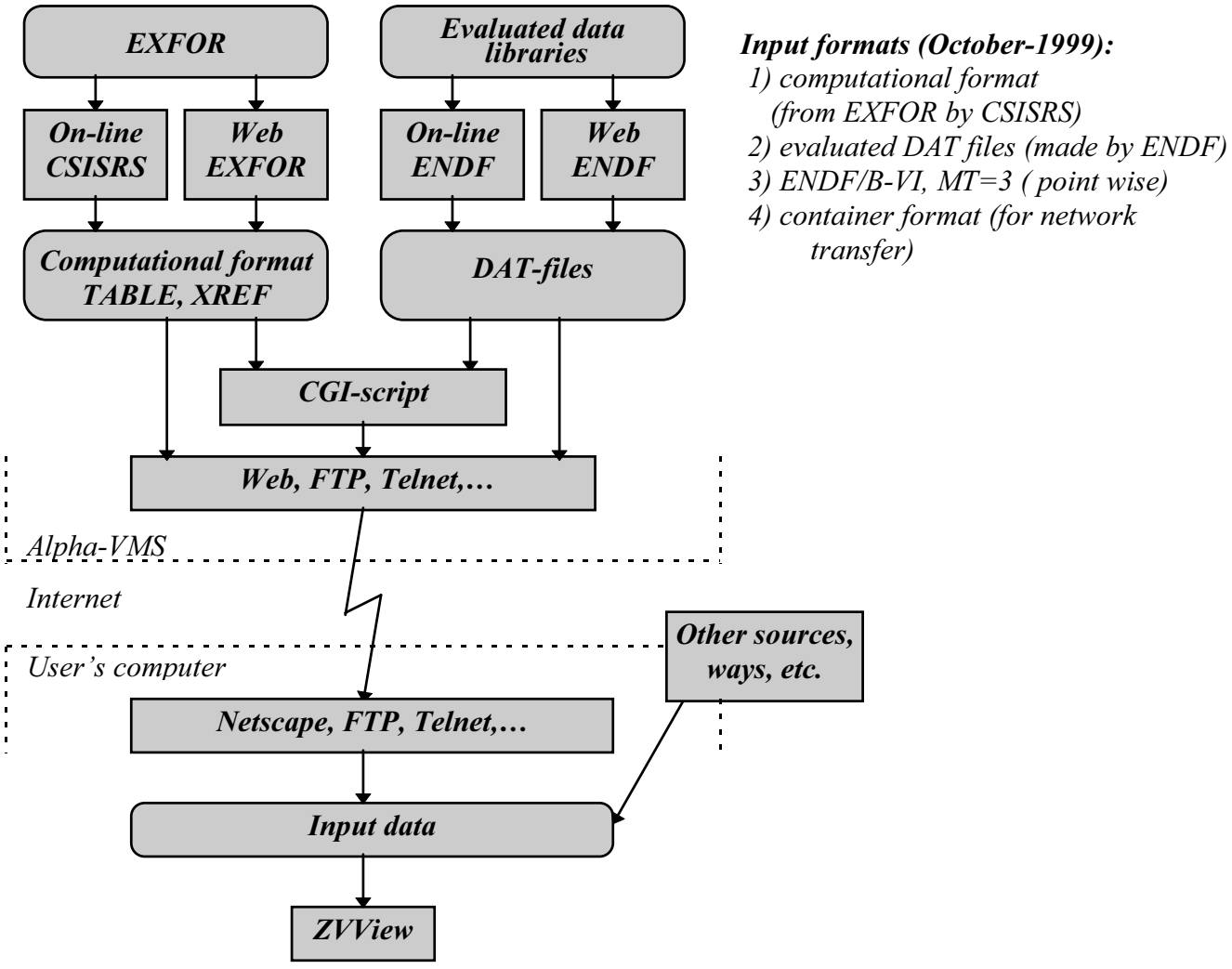
Design



ZVView can be used through Internet as a helper-application on local machine under browser (Netscape, MS-Explorer). For this purpose special ("Container") format of data was defined. This format allows to combine several data files in different formats in a single file.

Resent development in collaboration with NNDC (BNL, USA) coupled Web EXFOR and ENDF retrieval system based on Alpha-VMS with ZVView to display retrieved data on local computer. The combination of nice interface provided by modern browsers, remote Web retrieval system, data transfer via network to local computer under browser control, and automatically running ZVView gives to users easy to use and very convenient tool to display and analysis of data.

ZVView input data



In general, the idea to use ZVView as a helper under Internet browsers on various platforms can be also used for the design of various "Atlases" ("Catalogues", "Hand-books") containing nuclear physics information in Web style with interactive plots. This information service can be used either via Internet or locally. In particular, ZVView can be expanded to work as a part of user interface to database needed for PGAA that is being discussed in this CRP meeting.

Office of the Chief Engineer
Atomic Energy of Canada Limited

1999 August 12

To: Participants of CRP
From: Aslam Lone

CRP - Development of Database for Prompt Gamma-ray Activation Analysis

I was asked to provide recommendation or suggestion for this important endeavor.
Let me start with a brief history of the catalogue we published in ANDT
The catalogue "Prompt gamma rays from thermal-neutron capture" ADNDT 26(1981) was based on the data published in the open literature between 1968 and March 1980. The scope was set to satisfy needs of the technology as well as editorial policies of the ADNDT journal.

The energy of the gamma rays were computed from a weighted average of the energies reported by various authors. The standard deviation of the mean energy was generated but was not listed in the data tables because of the space limitation or lack of the availability of the quantitative information on individual gamma-rays.

The gamma -ray intensity adopted was an unweighted average primarily due to a lack of quantitative input data on uncertainties of the individual gamma-rays

The thermal neutron capture cross sections were adopted from BNL-325. It was recognized that for non-1/v elements, these cross section depend on the neutron spectral distribution in the beam (Cd ratio), so the facility dependent k_o values were not listed.

Bulk of the data included in the catalogue was from the MIT project. The attached files contain detailed information on the MIT reactor based (Ge(Li)-Na I) facility and data analysis including energy and intensity calibrations and determination of uncertainties. The energy was determined using lines of known energy present in the data from sample

holder and the background. The intensity was computed from , the observed counts using intrinsic and geometric efficiency factors that had been determined previous measurements, a correction for gamma-ray self absorption in the sample, calculation of total number of captures in the sample using measured total exposure and cross sections , and a correction for neutron flux depression in the sample. In the final results the intensities were re-normalized to match the observed total energy to the known binding energy of the element.

Suggestions for update of Data .

- update the data based with the new information published since 1980.
- include prominent short lived decay lines, as for Al
- The spectroscopic purity of the samples used should be examined to eliminate the gamma rays from impurities. The data in the existing catalogue show many low energy gamma rays that are potential contributions of sample impurities.
- list energy and intensity uncertainties of individual gamma-ray lines.
- maintain a generic data similar to the existing data base with intensities rather than k_0
- for generation of k values, list effective elemental cross sections for different types of neutron source energy distributions at various facilities. This would avoid repetition of the long tables. Individual groups would then be able to generate effective k_0 values relevant to their own facilities.
- list effective isotopic cross sections for industrially important materials. Again these would depend on energy spectrum of the neutron source.

Cc attachments (MIT documents)