

# Lawrence Berkeley National Laboratory

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Summary Report: First Research Coordination Meeting on Reference Database for Neutron Activation Analysis

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### **Authors**

Firestone, Richard B.  
Trkov, Andrej

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**Summary Report**

**First Research Coordination Meeting on**

**Reference Database for Neutron Activation Analysis**

IAEA Headquarters  
Vienna, Austria

3-5 October 2005

Prepared by

Richard B. Firestone  
Lawrence Berkeley National Laboratory  
University of California  
Berkeley, USA

and

Andrej Trkov  
IAEA Nuclear Data Section  
Vienna, Austria

October 2005

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IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Nuclear Data Section  
International Atomic Energy Agency  
PO Box 100  
Wagramer Strasse 5  
A-1400 Vienna  
Austria

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Richard B. Firestone  
Lawrence Berkeley National Laboratory  
University of California  
Berkeley, USA

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Andrej Trkov  
IAEA Nuclear Data Section  
Vienna, Austria

**Abstract**

Potential problems associated with nuclear data for neutron activation analysis were identified, the scope of the work to be undertaken was defined together with its priorities, and tasks were assigned to participants. Data testing and measurements refer to gamma spectrum peak evaluations, detector efficiency calibration, neutron spectrum characteristics and reference materials analysis.

October 2005



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## 1. Background

Due to its selectivity and sensitivity, neutron activation analysis (NAA) occupies an important place among the various analytical methods. It has proven to be a powerful non-destructive analytical technique for concentrations at or below the  $\mu\text{g/g}$  range, while up to 60 elements can be determined performing two irradiations and several gamma-spectrum measurements after different decay periods. The main fields of NAA application are analytical chemistry, geology, biology, and the life and environmental sciences. Its accuracy, the virtual absence of matrix effects and the completely different physical basis when compared to other analytical techniques, make it particularly suitable for the certification of candidate reference materials (RMs), providing e.g. the bulk of the literature data on the standard RMs of the National Institute of Standards and Technology and reference materials of the International Atomic Energy Agency.

The  $k_0$  standardisation method of NAA ( $k_0$ -NAA), a concept launched in 1975, can be interpreted as an absolute standardisation method. It relies on  $k_0$  and  $Q_0$  factors and a few other parameters that are composite constants derived from the basic nuclear data. In practice, they are usually determined by direct measurements, partly because equivalent constants derived from the basic data are often discrepant.

The aim of the Co-ordinated Research Project (CRP) on the Reference Database for Neutron Activation Analysis is to improve the status of the database of nuclear constants for  $k_0$ -NAA, to contribute to nuclear structure and decay data and to remove or reduce some of the discrepancies that exist between the integral constants and values derived from differential data.

The INDC Committee reviews the programme of the IAEA-NDS, and has endorsed the CRP at their meeting held in May 2002. A complementary project is in progress at NAPC-Industrial Applications and Chemistry Section on “ $k_0$ -IAEA Software Development for Neutron Activation Analysis”. This software package is chosen as the reference analysis tool for the current CRP.

The first Research Co-ordination Meeting (RCM) was held at the Agency Headquarters on 3-5 October 2005. The report below is a summary of the conclusions from that meeting.

## 2. Presentations

### A. Trkov, IAEA-NDS

The objectives of the CRP were re-iterated, namely:

- to improve database of nuclear constants for  $k_0$  NAA (improved  $k_0$  library),
- to improve consistency between integral and differential data (activation cross-section library),
- to contribute to nuclear structure and decay data (EGAF database),
- to extend applicability of  $k_0$  NAA.

Methods and procedures will be investigated for detector calibration, neutron spectrum characterization and gamma-spectrum processing methods. The nuclear database of integral constants will also be reviewed, performing new measurements as required.



**F. De Corte, Ghent University, Belgium**

A historical overview and the milestones in the most significant advances of the method were presented, explaining how the database was assembled and verified. Such information is essential for planning new measurements in order to generalize and improve the database.

**R. Jačimović, Institute Jožef Stefan, Ljubljana, Slovenia**

The  $k_0$ -method was introduced at the Jožef Stefan Institute (JSI) in Ljubljana at the end of 1988. Since then all recommended procedures for applying  $k_0$ -standardization method using TRIGA Mark II reactor have been implemented. The validation of the  $k_0$  method was established via the analysis of different reference and certified reference materials issued by the IAEA, NIST, BCR and IRMM. Up to now, relevant investigations for the CRP were done as follows: accurate determination of neutron spectrum parameters ( $f$  and  $\alpha$ ) in different irradiation channels, time-dependence of the neutron flux in different irradiation channels of the TRIGA reactor, neutron flux gradients (axial and radial) inside the irradiation channels, azimuthal variation of the neutron flux in the carousel facility (CF) of the TRIGA reactor, verification of Monte Carlo calculation of the neutron flux in CF, burn-up effects for some nuclides and systematic errors in the procedure for full-energy peak detection efficiency ( $\epsilon_p$ ) for an HPGe detector.

**B. Smodiš, Institute Jožef Stefan, Ljubljana, Slovenia**

Elements were identified that have incomplete information on uncertainties in their nuclear data. These should be addressed with high priority so that error propagation in routine measurements can be carried out correctly.

**S.A. Jonah, Ahmadu Bello University, Nigeria**

A description of the Nigerian MNSR (NIRR-1) and the experimental facilities was provided. Special mention was made of the current status of the facilities used for NAA by the relative method. In this regard, experimental procedures developed for sample analyses by the conventional method for over 30 elements were described. Measured neutron spectrum parameters required for the applicability of the  $k_0$ -standardization method were provided. The group's contribution to the CRP will be in the improvement of methodologies for determination of neutron spectrum parameters, measurement of some nuclear constants and the testing of the  $k_0$ -IAEA software.

**Maria Arribere, Centro Atomico Bariloche, Argentina**

The main goals of the group within this CRP are:

- i) perform core modeling by using Monte Carlo techniques,
- ii) perform flux characterization in the RA-6 irradiation positions through activity measurements and computational deterministic and statistical modelling,
- iii) use characterized irradiation channels to perform measurements of nuclear parameters of interest in NAA using the  $k_0$  method,
- iv) use characterized irradiation channels to measure resonance integrals and thermal cross sections of isotopes where both the ground and metastable states are formed, using the methodology developed at the laboratory that has already been applied to threshold reactions.

### **Richard Firestone, Lawrence Berkeley National Laboratory, Berkeley CA, USA**

Neutron activation analysis  $k_0$  data will be compared with gamma-ray transition probabilities from the ENSDF and DDEP decay data files and with data from the EGAF  $k_0$  file. New adopted decay,  $k_0$  and cross-section data will be added into EGAF.

### **Zsolt Revay, KFKI, Budapest**

In-beam activation technique is an excellent tool for measuring  $k_0$  factors using pure thermal neutrons, and also for studying isotopes with short half-lives. The calculation of self-shielding is also simple in beam geometry. Moreover, when the activation is performed in a cold neutron beam, the effects of resonances disappear. A series of measurements have been started at the Prompt Gamma Activation Analysis facility of the Budapest Research Reactor to re-determine  $k_0$  factors in the cold neutron beam. For a series of elements (like Na, Al, F, Mn), the decay peaks proved to be strong enough to analyze them in the usual prompt-gamma spectra. For weaker peaks the chopped-beam techniques is appropriate to separate the decay peaks from the prompt gamma spectrum. The elements from the priority list will be measured with either technique. The neutron spectrum was determined at the PGAA facility with time-of-flight technique using the beam chopper, and this will be done every time the beam configuration is changed. This information is used in the determination of effective  $g$  factors for nuclides such as  $^{147}\text{Gd}$ ,  $^{113}\text{Cd}$ , etc. This project is already going on.

## **3. Proficiency test**

The purpose of the proficiency test is to ensure that irradiation facilities and analysis software of the participants contributing experimental data will produce consistent results.

Proficiency tests will involve detector calibration, peak area determinations and neutron spectrum characterizations. Analysis will be done with  $k_0$ -IAEA software and other methods that may be available to the participants.

### **3.1. Gamma spectrum peak evaluation test**

The coordinator for the peak evaluation test will be Menno Blaauw. He will provide standard spectra for the purpose. Participants will submit results to the coordinator who will summarize the contributions at the next meeting.

### **3.2. Detector efficiency calibration**

The coordinator for the efficiency calibration will be Zsolt Revay. He will provide standard calibration spectra and calibration data. Participants will submit the specified results to the coordinator who will summarize the contributions at the next meeting.

### **3.3. Neutron spectrum characterization**

The coordinator for neutron spectrum characterization will be Andrej Trkov. Monitoring material from the  $k_0$ -IAEA package will be used by all participants for spectrum characterization of their irradiation facility. In addition, Frans De Corte will provide recommendations for other candidate materials that have suitable capture and threshold reactions.

The participants will be expected to determine  $f$  and  $\alpha$  by conventional methods. If available, participants will also provide neutron spectra in 640 group structure from statistical model

calculations or from direct measurements. Spectrum characterization results will be sent to Andrej Trkov for further analysis.

### 3.4. Materials analysis test

All participants will perform a materials analysis test. Frans De Corte will review the availability and appropriateness of using synthetic multi-element standard materials (SMELS) or a suitable substitute. He will also look into the future possibility of SMELS production. Maria Arribere will collect the results of the materials analysis test and write a report for the next RCM meeting.

## 4. $k_0$ -IAEA software package

Recently introduced features of the  $k_0$ -IAEA software were discussed. Menno Blaauw will distribute the latest update of  $k_0$ -IAEA software to all participants.

## 5. Nuclear Data

Definitions of nuclear constants and their relation to differential data will also be provided by Andrej Trkov, who will also calculate a) self-shielding factors as a function of the Bondarenko dilution cross section, b) effective resonance energies and c) effective  $g$ -factors from the same data source.

If changes in the  $k_0$  database are needed, all constants for a nuclide will be reviewed.

Data currently in the  $k_0$  database will be compared with equivalent data from other sources. The purpose of this intercomparison exercises is to identify discrepant data that may require re-evaluation or new measurements.

$P_\gamma$  and  $k_0$  values will be compared and evaluated for the EGAF library by Richard Firestone. Data from the  $k_0$  database, ENSDF, DDEP, EGAF and the literature will be considered.

Half-life data from the  $k_0$  database provided by Frans De Corte will be compared by Mark Kellett with values from the evaluated databases.

Andrej Trkov will compare  $Q_0$  values from the  $k_0$  database with IRDF-2002 and JEFF-3.1 activation library.

## 6. Criteria for determining priorities and scope of new measurements

Priorities for re-evaluation or re-measurement of constants for the  $k_0$  database have been elaborated as follows.

### Nuclides with discrepant data

$^{96}\text{Zr}$	discrepant measurements of $Q_0$
$^{94}\text{Zr}$	complementary to $^{96}\text{Zr}$
$^{127}\text{I}$	5% discrepancy in $k_0$
$^{23}\text{Na}$	different $k_0$ for 2 lines that should be the same

<sup>27</sup> Al	2σ discrepancy between recommended and $k_0$ measured at KFKI
<sup>131</sup> Ba	inconsistent measurements for $k_0$ and $Q_0$
<sup>138</sup> Ba	inconsistent measurements for $k_0$ and $Q_0$
<sup>121</sup> Sb	discrepancy in $k_0$ , $Q_0$ resulting in different concentrations from 2 isotopes
<sup>123</sup> Sb	discrepancy in $k_0$ , $Q_0$ resulting in different concentrations from 2 isotopes

### Important monitor materials

<sup>64</sup>Zn  
<sup>68</sup>Zn

### Non-1/ν absorbers

List will be provided by Zsolt Revay.

### Nuclides with high effective resonance energy $E_r$

$Q_0$	$E_r$	Isotope	$\sigma_0$
5.93	4300	<sup>90m</sup> Y	0.001
5.05	6260	<sup>95</sup> Zr	0.0499

### Lower priority ( $Q_0 < 5$ )

1.12	2280	<sup>37</sup> S	0.15
1.14	1040	<sup>64</sup> Cu	2.17
1.908	2560	<sup>65</sup> Zn	0.76
2.38	3540	<sup>75m</sup> Ge	0.17
1.57	3540	<sup>75</sup> Ge	0.34
1.8	2950	<sup>131</sup> I	6.2
1.2	1540	<sup>143</sup> Ce	0.95

Additional candidate materials for review will be identified by the intercomparison exercise described in Section 5. Also, Zsolt Revay will consult with Greg Kennedy whether any additional materials need to be included in the list.

There was general consensus that voluntary contributions from qualified researchers or laboratories will be valued for analysis and inclusion in the final database as appropriate. The authors will be acknowledged in the final document.

The web page is maintained by NDS for efficient exchange of information between interested parties, but is not advertised from the main web page. None of the participants objected to making the address known to potential contributors who are not formally CRP participants.

## 7. Next meeting

The next RCM meeting is scheduled in Spring 2007, the venue and the date to be decided.



## International Atomic Energy Agency

## First Research Co-ordination Meeting on

*“Reference Database for Neutron Activation Analysis”*

IAEA Headquarters, Vienna, Austria

3-5 October 2005

Meeting Room ACV-03-250

**LIST OF PARTICIPANTS****ARGENTINA**

Maria A. Arribere  
 Centro Atomico Bariloche  
 Comision Nacional de Energia Atomica  
 Bustillo 9500  
 8400 Bariloche  
 Rio Negro  
 Tel: +54 (2944) 445240  
 Fax: +54 (2944) 445299  
 E-mail: arribere@cab.cnea.gov.ar

**BELGIUM**

Frans De Corte  
 Ghent University  
 INW-Proeftuinstraat 86  
 B-9000 Gent  
 Tel: +32 9 2646627  
 Fax: +32 9 2646699  
 E-mail: [frans.decorte@Ugent.be](mailto:frans.decorte@Ugent.be)

**HUNGARY**

Zsolt Revay  
 Institute of Isotopes  
 Chemical Research Centre  
 Hungarian Academy of Sciences  
 Department of Nuclear Research  
 H-1121 Budapest, Konkoly Thege Str. 29-33  
 Tel: +36 1 392 2539  
 Fax: +36 1 392 2584  
 E-mail: revay@iki.kfki.hu

**NIGERIA**

Sunday A. Jonah  
 Centre for Energy Research and Training  
 (CERT)  
 Ahmadu Bello University  
 PMB 1014 Zaria  
 Tel: +234 69 550397  
 Fax: +234 69 550737  
 E-mail: jonahsa2001@yahoo.com

**SLOVENIA**

Radojko Jačimović  
 Laboratory for Radiochemistry  
 Department of Environmental Sciences  
 Institute Jožef Stefan  
 Jamova 39  
 SI-1000 Ljubljana  
 Tel: +386 1 5885353  
 Fax: +386 1 5885346  
 E-mail: radojko.jacimovic@ijs.si

**UNITED STATES OF AMERICA**

Richard B. Firestone  
 Lawrence Berkeley National Laboratory  
 University of California  
 1 Cyclotron Road, M/S 88RO192  
 Berkeley, CA 94720-8101  
 Tel: +1 510 486 7646  
 Fax: +1 510 486 5757  
 E-mail: RBF@lbl.gov

**ADVISOR****THE NETHERLANDS**

Menno Blaauw  
 Reactor Institute Delft  
 Facilities & Services Dept.  
 Mekelweg 15  
 NL-2629 JB Delft  
 Tel: +31 15 278 3538  
 Fax: +31 15 278 8430  
 E-mail: m.blaauw@tnw.tudelft.nl

**OBSERVER****SLOVENIA**

Borut Smodiš  
 Institute Jožef Stefan  
 Jamova 39  
 SI-1000 Ljubljana  
 Tel: +386 1 2885450  
 E-mail: Borut.Smodis@ijs.si

**IAEA:**

Andrej Trkov  
Nuclear Data Section  
Division of Physical and Chemical Sciences  
Room A2316  
Tel: +43 1 2600-21712  
Fax: +43 1 26007  
E-mail: A.Trkov@iaea.org

Alan L. Nichols  
Nuclear Data Section  
Division of Physical and Chemical Sciences  
Room A2313  
Tel: +43 1 2600-21709  
Fax: +43 1 26007  
E-mail: A.Nichols@iaea.org

Mark A. Kellett  
Nuclear Data Section  
Division of Physical and Chemical Sciences  
Room A2319  
Tel: +43 1 2600 21708  
Fax: +43 1 26007 21708  
E-mail: M.A.Kellett@iaea.org

Matthias Rossbach  
Industrial Applications and Chemistry Section  
Division of Physical and Chemical Sciences  
Room A2370  
Tel: +43 1 2600 21750  
Fax: +43 1 26007 21750  
E-mail: M.Rossbach@iaea.org

Chushiro Yonezawa  
Nutritional and Health Related Environmental  
Studies Section  
Division of Human Health  
Room A2424  
Tel: +43 1 2600 21652  
Fax: +43 1 26007 21652  
E-mail: C.Yonezawa@iaea.org



International Atomic Energy Agency

**First Research Coordination Meeting on**

*Reference Database for Neutron Activation Analysis*

IAEA Headquarters, Vienna, Austria

3 – 5 October 2005

Meeting Room ACV-03-250

**AGENDA**

**Monday, 3 October**

- 08:30 – 09:20**    **Registration** (IAEA registration desk, Gate 1)
- 09:30 – 10:00**    **Opening Session**  
 Opening by Mr. N. Ramamoorthy, Director-NAPC  
 Introductory remarks (A. Trkov)  
 Election of Chairman and Rapporteur  
 Discussion and adoption of the Agenda (Chairman)  
 Election of task co-ordinators
- 10:00 – 11:00**    *Coffee break and Administrative Matters*
- 11:00 – 12:20**    **Session 1: Presentations by participants**  
 (max: 15 min per presentation + 5 min discussion)
- 12:20 – 14:00**    *Lunch*
- 14:00 – 15:30**    **Session 2: Presentations by participants (cont'd.)**  
 (max: 15 min per presentation + 5 min discussion)  
 General Discussion
- 15:30 – 16:00**    *Coffee break*
- 16:00 – 17:30**    **Session 3: Definition of a proficiency test case**  
 Detector calibration  
 Neutron spectrum determination / monitor reactions  
 Gamma spectrum analysis  
 Processing of results  
 General Discussion
- 17:30 onwards**    *Social event*



## Tuesday, 4 October

- 08:30 – 09:30**    **Session 4: Neutron spectrum determination**  
Conventional methods of NAA  
Spectrum unfolding  
Direct measurements  
Computational methods  
General Discussion
- 09:30 – 10:15**    **Session 5:  $k_0$ -IAEA software package**  
Detector calibration utilities  
Spectrum processing utilities  
Scope of software intercomparison with other products  
Software extensions  
General Discussion
- 10:15 – 10:45**    *Coffee break*
- 10:45 – 12:15**    **Session 6: Specific features**  
Items drafted by chairman
- 12:15 – 14:00**    *Lunch*
- 14:00 – 15:30**    **Session 7: Nuclear constants in relation to differential data**  
Relation between integral and differential data  
Neutron self-shielding  
Effective resonance energy  
Gamma emission probabilities
- 15:30 – 16:00**    *Coffee break*
- 16:00 – 17:30**    **Session 8: Criteria for determining the scope of new measurements**  
Needs and priorities  
Available facilities  
Available manpower

## Wednesday, 5 October

- 08:30 – 10:15**    **Session 9: Task assignment and drafting of summary report**
- 10:15 – 10:45**    *Coffee break*
- 10:45 – 12:15**    **Session 10: Task assignment and drafting of summary report**
- 12:15 – 14:00**    *Lunch*
- 14:00 – 15:30**    **Session 11: Review of the summary report**
- 15:30**            **Closing of the meeting**

## GUIDELINES

### General:

- Please, check the NAA CRP web page <http://www-nds.iaea.org/naa/index.html> frequently for announcements and up-to-date information.
- For all administrative queries please contact Ms. Janet Roberts on [J.Roberts@iaea.org](mailto:J.Roberts@iaea.org).
- For technical matters please contact the technical officer of the project Andrej Trkov on [A.Trkov@iaea.org](mailto:A.Trkov@iaea.org) with a copy to Ms. Roberts.

### Presentations:

- Oral presentations at the meeting are deliberately short.
- The presentations should *not* describe details of the theoretical advances, but primarily inform other participants (not necessarily experts in the specific field) on your planned contribution to the CRP.

## TASK ASSIGNMENTS

Participant	Date	Task	Status
Menno Blaauw	11 July 2006	<b><u>Gamma spectrum peak evaluation test.</u></b> Coordinate activity.	
	5 Dec. 2005	Provide standard spectra for purpose to participants.	
All participants	30 April 2006	Submit results to coordinator.	
Menno Blaauw	Next RCM	Summarize contributions.	
Zsolt Revay	May 2006	<b><u>Detector efficiency calibration.</u></b> Coordinate activity. Provide standard calibration spectra and calibration data to participants.	
All participants	31 Oct 2006	Submit results according to specifications to coordinator.	
Zsolt Revay	Next RCM	Summarize contributions.	
Andrej Trkov	Next RCM	<b><u>Neutron spectrum characterization.</u></b> Coordinate activity.	
Frans De Corte	Dec. 2005	Provide recommendations for other candidate materials that have suitable capture and threshold reactions.	Done
All participants	Dec. 2006	Monitoring material from the $k_0$ -IAEA package to be used by all participants for spectrum characterization of their irradiation facility, in addition to any other available monitor materials. Determine $f$ and $\alpha$ by conventional methods.	
All participants	Dec. 2006	If available, also provide neutron spectra in 640 group structure from statistical model calculations or from direct measurements. To be sent to Andrej Trkov for further analysis.	
Andrej Trkov	Next RCM	Further analysis of spectrum characterization results.	
Andrej Trkov	Next RCM	Summarize contributions.	
Maria Arribere	Next RCM	<b><u>Materials analysis test.</u></b> Coordinate activity.	
All participants	Next RCM	To perform a materials analysis test.	

Participant	Date	Task	Status
Frans De Corte	Dec. 2005	<u>Materials analysis test (cont.)</u> To review the availability and appropriateness of using synthetic multi-element standard materials (SMELS) or a suitable substitute. To look into the future possibility of SMELS production.	Done
Maria Arribere	Next RCM	Collect the results and write a report.	
Menno Blaauw	12 Dec 2005	<u><math>k_0</math>-IAEA software package.</u> Distribute the latest update of $k_0$ -IAEA software to all participants.	
Andrej Trkov	7 Jan 2006	<u>Nuclear Data</u> Provide definitions of nuclear constants and their relation to differential data. Calculate a) self-shielding factors as a function of the Bondarenko dilution cross section, b) effective resonance energies and c) effective g-factors from the same data source.	Done
	Sept. 2006	Data currently in the $k_0$ database to be intercompared with equivalent data from other sources to identify discrepant data that may require re-evaluation or new measurements	
Richard Firestone	Dec. 2006	Compare and evaluate $P_\gamma$ and $k_0$ values for the EGAF library. Data from the $k_0$ database, ENSDF, DDEP, EGAF, and the literature to be considered.	
Frans De Corte	Oct. 2005	Provide half-life data from the $k_0$ database.	
Mark Kellett	Jan. 2006	Compare half-life data from the $k_0$ database with values from the evaluated databases.	
Zsolt Revay	28 Feb. 2006	<u>Criteria for determining priorities and scope of new measurements.</u> Consult with Greg Kennedy whether any additional materials need to be included in the list.	





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Nuclear Data Section  
International Atomic Energy Agency  
P.O. Box 100  
A-1400 Vienna  
Austria

e-mail: [services@iaecand.iaea.org](mailto:services@iaecand.iaea.org)  
fax: (43-1) 26007  
cable: INATOM VIENNA  
telex: 1-12645  
telephone: (43-1) 2600-21710

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