Proposal for a Co-ordinated Research Project (CRP)

1. *Title of CRP*: Reference Database for Neutron Activation Analysis

2. *Background Situation Analysis (Rationale/Problem Definition)*

Neutron activation analysis is a nuclear technique for the analysis of sample composition whereby the sample is irradiated in a neutron field and composition is determined by identifying characteristic gamma radiation emitted by the activation products. The method has a broad range of applications due to its high sensitivity and the multi-elemental nature of the results; namely, from a single measurement of a sample the concentrations of a whole range of elements can be determined, even when present in small amounts. The technique relies on changes that occur in a nucleus after interacting with the incident particle (neutron). After neutron interaction the residual nucleus returns to the ground state by the emission of characteristic gamma radiation, which carries the "signature" of the element. Analysis of these gamma rays (during sample irradiation) is the basis for the so-called Prompt-gamma Neutron Activation Analysis (PGAA). Residual nuclei themselves are very often radioactive. On decay the decay products are formed, which emit characteristic gamma rays when settling to their ground states. Analysis of the gamma rays of decay products (some time after irradiation) is the basis for the conventional Neutron Activation Analysis (NAA), which is the subject of the present CRP.

Correct interpretation of the measured gamma spectra requires good knowledge of the reaction mechanisms, particle transport and accurate nuclear constants that describe them. Validity of these constants is limited to systems with neutron spectrum characteristics consistent with the basic assumptions underlying the definitions. Understanding these definitions and the assumptions is the key to a reliable application of the method and possible extension to system with different neutron spectrum characteristics.

Integral nuclear constants for NAA have been measured experimentally and published in the literature by various authors. Starting from the basic definitions of the integral constants and using cross sections from evaluated nuclear data files it is often found that significant discrepancies exist, compared to measured values. They may be caused by deficiencies in the energy-dependent cross section data, systematic errors in the experimental measurements or inadequate knowledge of the neutron spectrum characteristics of the irradiation facility where measurements are performed. Removal of such discrepancies is one of the objectives of the project. The outputs will be: an improved database of integral nuclear constants for NAA, an improved library of energy-dependent cross sections for some reactions (consistent with integral constants) and a contribution to the nuclear structure database. The outcome will be the improved accuracy and reliability of NAA, possibility of extension to irradiation facilities with different spectral characteristics and general improvements in the neutron dosimetry techniques due to the improvements in the cross section and nuclear structure databases.

The CRP will address experimental measurements and analysis in a unified approach, including detector calibration, gamma spectrum analysis, neutron spectrum characterisation by activation measurements and by computational methods. This should help to resolve any discrepancies and contribute to the understanding of the mechanisms involved.

The INDC Committee, which reviews the programme of the IAEA-NDS has endorsed the proposed CRP at the meeting held in May 2002.

A CRP has been completed recently, which addressed the data needs for PGAA. The database is available on the NDS web site http://www-nds.iaea.org/pgaa/ and the TECDOC is to be released as soon as clearance from the publishing committee of the IAEA is obtained. The presently proposed CRP is a complementary activity aimed at improving the database for the conventional NAA.

A project is in progress at NAPC-Industrial Applications and Chemistry section on "k_0 Software Development for Neutron Activation Analysis". There is close collaboration with the project officer in the preparatory stages of the proposed CRP.

A workshop on "Nuclear Data for Activation Analysis" is organised jointly by ICTP and IAEA. Further information is available in the Calendar for 2005 on the ICTP web site http://www.ictp.trieste.it/. In this workshop the above-mentioned k_0-IAEA software will be presented. It will also give an opportunity to establish links with potential participants and contributors to the CRP.

3. *Overall Objective*

The overall objective of the IAEA CRP on the Reference Database for Neutron Activation Analysis is:

- To improve the database of integral nuclear constants for NAA.
- To improve consistency between energy-dependent cross sections and integral constants used in NAA.
- To contribute to the nuclear structure database.

4. *Specific Research Objective (Purpose)*

Activities within the CRP will include:

- Re-measuring of nuclear constants for activation analysis on different facilities, paying special attention to the determination of spectral characteristics of the irradiation facilities and focusing on nuclides for which there exist large discrepancies in the measurements or in comparison with constants derived from energy-dependent cross sections.
- Compilation of the newly measured data into the library of nuclear constants for activation analysis.
- Validation of the new library by the analysis of reference materials.
- Use of the experimental data to obtain nuclear structure information and updating of the EGAF library.
- Tracing of possible sources of discrepancies in equivalent constants derived from energy-dependent cross sections and scaling of the differential data, if applicable.
- Release of a consistent cross section file from which a consistent set of constants for activation analysis can be derived from the basic definitions.

5. *Expected Research Output (Results)*

The main output of the project will be new and improved database of integral nuclear constants for NAA, a set of evaluated cross section data files for selected nuclides consistent with the integral nuclear constants, updated nuclear structure EGAF file and the documentation of the details of the evaluation process, experimental data included in the evaluation, etc.

The basic data will be thoroughly checked for formal correctness and internal consistency.

The data will be distributed to the users through the Web and on CD-ROMs.

The new database of integral constants for NAA will improve the accuracy and reliability of NAA. Thorough understanding of the physical phenomena will allow extensions of the method to irradiation facilities with spectral characteristics that violate the assumptions implicit in the current usage of the method. As a by-product, a library of cross section data will be produced that will be consistent with the integral parameters. The nuclear structure file EGAF will also be extended by inclusion of the new data.

6. *Relationship to sub-programme objective*

The proposed CRP is directly related to the objective of the Sub-programme D1 – "Nuclear and Atomic Data" for years 2004-2005, namely: *To contribute to the safe and economic application of nuclear technologies in Member States by ensuring convenient access to accurate and reliable nuclear and atomic data for energy and non-energy applications.*

7. *Action Plan (Activities)*

Activity	***2005***	***2006***	***2007***	***2008***	***2009***
1. Constitute the CRP, select participants (finalize all by June 2005). Prepare CRP working plan via e-mail communication, plan work under individual research contracts and agreements and begin work	X				
2. Organize 1st RCM (November 2005) to discuss and co-ordinate plans for further work on measurements, evaluation, database assembly, verification and benchmarking.	X				
3. Organize 2nd RCM (Mar 2007) to review the results achieved, to discuss the recommendations on the evaluation methodology in view of preliminary benchmark results			X		
4. Organize 3rd RCM (final, September 2008) to consider and review the preliminary benchmarking results and discuss the details of the final presentation of the results				X	
5. Prepare and submit for publication the final report with the results of CRP; create Web access to the new database for activation analysis and prepare for data distribution on CD-ROMs (December 2008).				X	
6. Prepare the TECDOC for publication.					X

8. *Inputs*

(a) Financial Resources

Item	***2005***	***2006***	***2007***	***2008***	***2009***
Research Contracts	15,000	15,000	15,000		3,000
RCMs	20,000		20,000	20,000	
Publication					2,000
Total	**35,000**	**15,000**	**35,000**	**20,000**	**5,000**

Total for the CRP: $ 110,000

9. *Assumptions*

No outside factors, which could prevent the implementation of the proposed CRP, are foreseen at this time.

10. *Logical Framework*

Narrative Summary	***Objective Verifiable Indicators***	***Means of Verification***	***Important Assumptions***
Overall objectives: To provide improved database of nuclear constants for conventional NAA.	New database of nuclear constants for NAA produced.	Availability of the new database.	None
Specific objectives: Co-ordinate activities on new measurements and assembly of an improved database of nuclear constants	Reports prepared describing the measurements, their verification and partial validation.	Availability of reports.	National support provided to participants
Outputs: 1. Improved database of nuclear constants for NAA. 2. Database integrated into the K-IAEA software package, which is also an IAEA product. 3. Reports from the data verification and validation process.	New database of nuclear constants for NAA complete with documentation available on the web.	Review of the documentation.	None
Activities: 1) Constitute the CRP, select participants, prepare CRP working plan and begin the work.	1) Research contracts and Agreements awarded	1) Approval of Contracts and Agreements by PCC	1) Suitable proposals submitted
2) Organize 1st RCM to discuss and co-ordinate plans for further work on measurements, data analysis, verification and validation, on level of co-operation needed to come to consistent conclusions and first results obtained by participants.	2) 1st RCM held	2) RCM summary report, CRP Progress Reports	2) None
3) Organize 2nd RCM to review the results achieved, to discuss the recommendations on the methodology in view of preliminary validation results.	3) 2nd RCM held	3) RCM summary report, CRP Progress Reports	3) None
4) Organize 3rd (final) RCM to consider and review the validation results and to discuss the details of the final presentation of the results	4) 3rd RCM held	4) RCM summary report, CRP Progress Reports.	4) None
5) Prepare and submit for publication the final report with the results of CRP; create Web access to the database and prepare data for distribution on CD-ROMs	5) Database prepared and report submitted for printing	5) Database and documentation available	5) None

11. *Brief Summary for the Agency's Bulletin*

Neutron Activation Analysis (NAA) is a nuclear technique for the determination of elemental composition by analysis of the emitted gamma-ray spectra from sample nuclei after their interaction with incident neutron particles. The method is highly sensitive, and has a broad range of applications due to the multi-elemental nature of the results. Its accuracy depends on the correct interpretation of the measured gamma-ray spectra and requires good knowledge of the reaction mechanisms, particle transport and accurate nuclear constants that describe them. This CRP will contribute to a better understanding of the mechanisms involved, and the primary product will be an updated and considerably improved database of nuclear constants to enhance the accuracy and reliability of the method for sample analysis. After verification and validation studies, the database will be integrated into the IAEA k_0-software package for analysis of the NAA measurements, which is also an IAEA product.

Appendix 1

List of Potential Participants of the CRP
"Reference Database for Neutron Activation Analysis"

1. Belgium, Consultancy on past measurements (F. De Corte, Research Agreement).

2. Netherland, Consultancy on k0-IAEA software (M. Blaauw, Research Agreement).

3. Slovenia, Measurements in different irradiation channels of a TRIGA reactor, neutron spectrum determination by computational model (R. Jacimovic, Research **Contract**).

4. USA, Analysis of partial cross section data, insertion of nuclear structure data into the EGAF library (R. Firestone, Research Agreement).

5. Argentina, Measurements in different irradiation channels of the local reactor (S. Ribeiro or F. Leszczynski, Research **Contract**).

6. Hungary, Measurements in a well-thermalised neutron beam (Z. Revay, Research Agreement).

7. USA, Measurements in different irradiation channels of the local reactor, neutron spectrum determination by computational model (L. Griffin, Research Agreement or Technical Contract).

8. Three more participants (one research contract) – to be selected in March 2005.

Project Officer of the CRP:
Andrej Trkov
IAEA Nuclear Data Section
Wagramer Strasse 5
P.O. Box 100
A-1400 Vienna
Phone: +43 1 2600 21712
Fax: +43 1 26007
E-mail: A.Trkov@iaea.org