NAA Software

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Introduction

Two features of (n,γ) reactor NAA are making its standardization potentially easy and accurate:

1. **the high penetrability of matter for neutrons**
2. **existence of a delayed signal (besides the prompt gamma's).**

Hence, standard and sample can be excited simultaneously and induced signals of both can be measured successively after a suited time following the end of irradiation.

Introduction

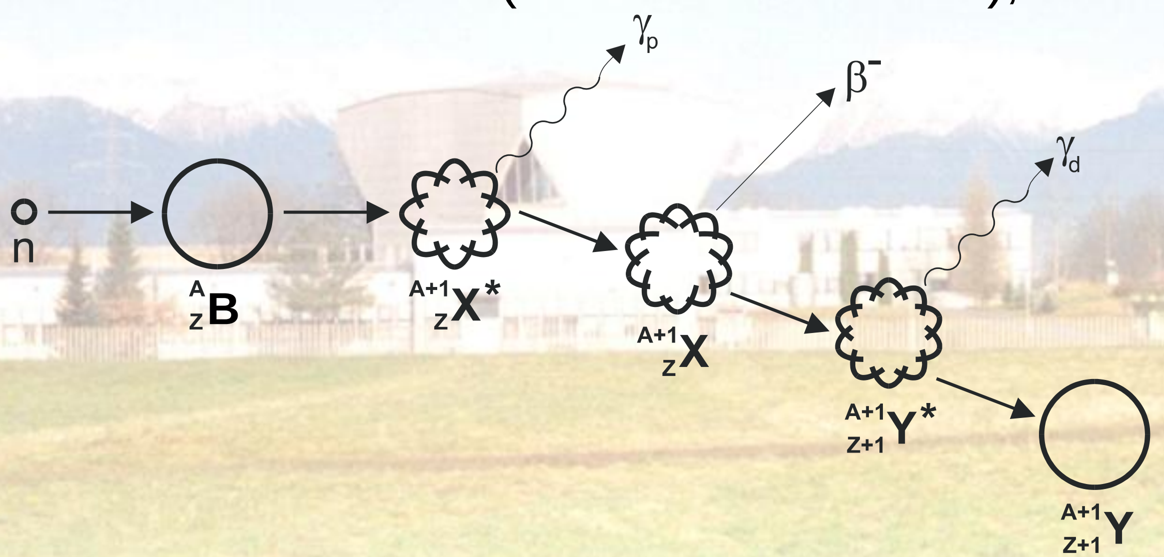
Other consequences:

- NAA is a bulk analysis method with multi-element capability (element concentration and measured signal is nearly matrix-independent).
- Matrix preparation can be kept simple.
- Treatment of sample (and standard) after irradiation is possible (enabling etching, dissolution, chemical separation - RNAA).
- High sensitivity (down to the 10^{-6}, 10^{-9} or even to the 10^{-12} g/g) attainable for many elements.
- Reference method for certification of new CRMs or RMs.

Introduction

Nuclear reactions: - direct ($B + a \rightarrow Y + b$); ~ 10^{-22} - 10^{-21} s

- meta stable ($B + a \rightarrow X^* \rightarrow Y + b$); ~ 10^{-16} - 10^{-14} s



[e. g. $n + {}^{197}_{79}Au \longrightarrow {}^{198}_{79}Au^* \longrightarrow {}^{198}_{79}Au \longrightarrow {}^{198}_{80}Hg^* \longrightarrow {}^{198}_{80}Hg$]

(γ_p, β^-, γ_d)

A typical (n,γ) reaction with β^- decay.

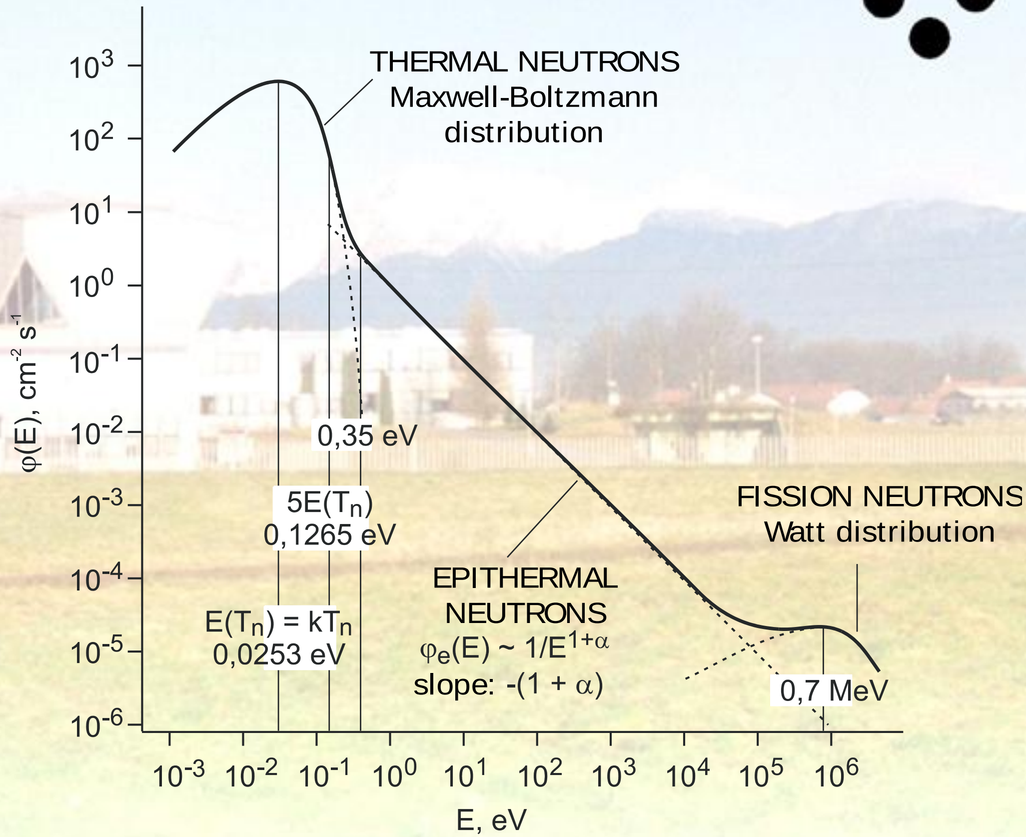
Introduction

- NAA - four techniques:
  - Prompt Gamma Neutron Activation Analysis (**PGNAA**) (usually with energies < 0.001 eV); prompt gammy rays (γ_p) emitted by the compound nucleus X^* are measured
  - Thermal Neutron Activation Analysis (**TNAA**); from reactions in a well-thermalised reactor spectrum, the decay gamma rays (γ_d) are measured
  - Epithermal Neutron Activation Analysis (**ENAA**); resonance reactions are utilised by using suitable filters to remove thermal neutrons from the reactor spectrum and measuring decay gamma rays
  - Fast Neutron Activation Analysis (**FNAA**); high-energy neutron sources are used without the presence of a moderator for slowing down the neutrons and gamma rays are measured.

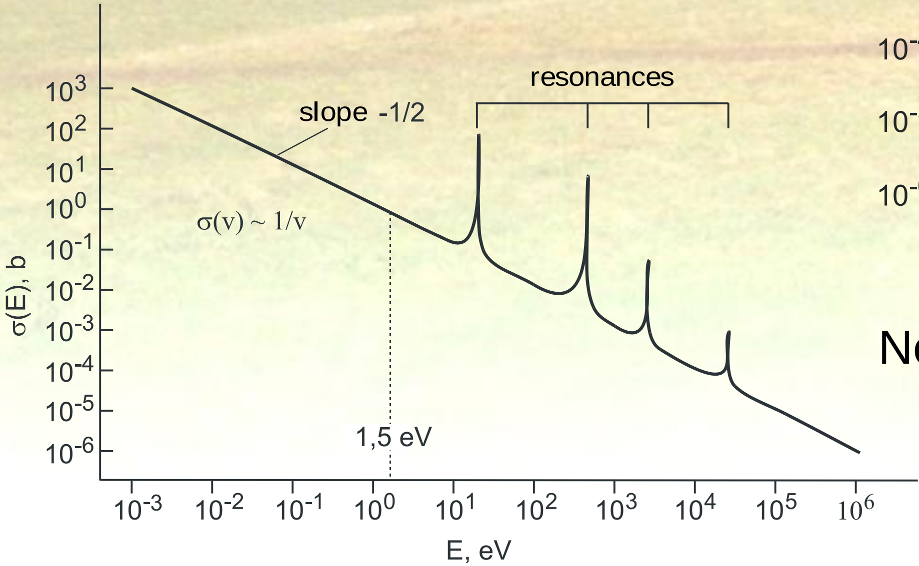
(n,γ) reaction rate

Specific reaction rate per target nuclide

$$R_X = \frac{R}{N_1} = \int_0^{\infty} \sigma(E)\varphi(E)\,dE$$

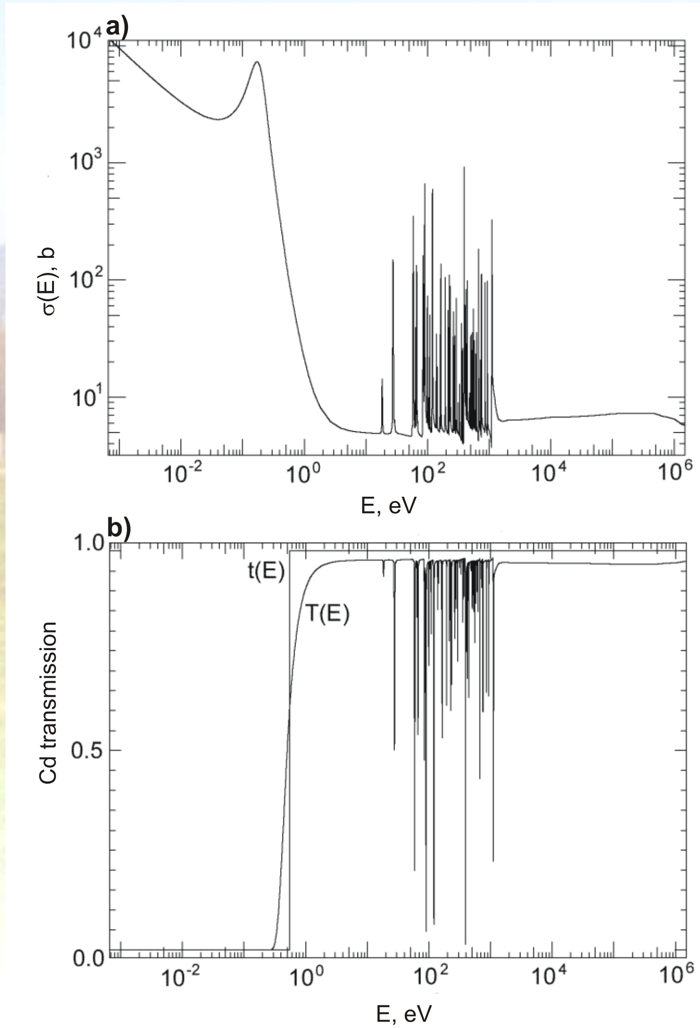


Neutron fluence rate distribution vs. E



Cross-section vs. E ($\sigma(v) \sim 1/v$)

(n,γ) reaction rate



Cd total cross section and Cd transmission function T(E) for 1 mm Cd

Hogdahl convention:

$$R_X = \int_0^{v_{Cd}} \sigma(v)\,\varphi'(v)\,dv + \int_{E_{Cd}}^{E_2} \sigma(E)\,\varphi(E)\,dE = R_{X,th} + R_{X,e}$$

- all (n,γ) reactions are as follows:

$$\sigma(v) \propto 1/v$$

- E_{Cd} = 0.55 eV

$$R_X = \sigma_0\, v_0\, n_{th} + \varphi_e\, I_0(\alpha) = \sigma_0\, \varphi_{th} + \varphi_e\, I_0(\alpha)$$

with: $\sigma_0 = \sigma(v_0)$ at reference velocity v_0 =2200 m s^{-1}, $\varphi_{th} = v_0\, n_{th}$ **fluence rate for thermal neutrons**, n_{th} – thermal neutron density **and**

$$I_0(\alpha) = (1eV)^{\alpha} \int_{E_{Cd}}^{E_2} \frac{\sigma(E)\,dE}{E^{1+\alpha}}$$

resonance integral for epithermal part of spectra

(n,γ) reaction rate

For better adjustment of (n,γ) reaction rate in Hogdahl convention it is necessary to introduce some correction factors:

- G_{th} - thermal neutron self-shielding (nucleus density)
- G_e - epithermal neutron self-shielding (density + resonance parameters)
- F_{Cd} - Cd transmission factor for epithermal neutrons

$$R_X = G_{th}\,\varphi_{th}\,\sigma_0 + G_e\,\varphi_e\,I_0(\alpha)$$

Cd-ratio:

$$R_{Cd} = F_{Cd}\,R^*_{Cd} = 1 + \left(\frac{G_{th}\,f}{G_e\,Q_0(\alpha)}\right)$$ with $$f = \frac{\varphi_{th}}{\varphi_e}$$ and $$Q_0(\alpha) = \frac{I_0(\alpha)}{\sigma_0}$$

with R_{Cd}^* - measured Cd ratio:

$$R^*_{Cd} = \frac{\int_0^\infty \sigma(E)\,\varphi(E)\,dE}{\int_0^\infty T(E)\,\sigma(E)\,\varphi(E)\,dE} = \frac{\int_0^{E_2} \sigma(E)\,\varphi(E)\,dE}{F_{Cd}\int_{E_{Cd}}^{E_2} \sigma(E)\,\varphi(E)\,dE}$$

Activation equation

$$N_1^0 = \frac{w N_A \Theta}{M}$$

$$\frac{dN_1}{dt'} = -N_1 R_{X,1}$$

$$N_1 = N_1^0 \, e^{-R_{X,1} t'}$$

taking into account the removal of nuclei of the nuclide produced

$$\frac{dN}{dt'} = N_1 R_{X,1} - N(\lambda + R_N) = R_{X,1} N_1^0 \, e^{-R_{X,1} t'} - N(\lambda + R_N)$$

$$N = \frac{N_1^0 \; R_{X,1} \, e^{-R_{X,1} t_{irr}}}{(\lambda + R_N - R_{X,1})} \left(1 - e^{(R_{X,1} - \lambda - R_N)\, t_{irr}}\right)$$

$$N = \frac{N_1^0 \; R_{X,1}}{\lambda} \left(1 - e^{-\lambda t_{irr}}\right)$$

not taking into account the removal of nuclei of the nuclide produced

Burn-up factor

$$F_{burn} = \frac{\lambda \; e^{-R_{X,1} t_{irr}} \left(1 - e^{(R_{X,1} - \lambda - R_N)\, t_{irr}}\right)}{(\lambda + R_N - R_{X,1}) \left(1 - e^{-\lambda \, t_{irr}}\right)}$$

N^0_1 - initial number of irradiated nuclei in the target
N_1 - number of target nuclide
N - number of radionuclide
w – mass of the investigated element
N_A- Avogadro constant=6.022045 10^{23} mol^{-1}
M - molar mass
Θ - isotopic abundance
λ - decay constant = *ln(2)/*$T_{1/2}$
t_{irr} - irradiation time
$R_{X,1}$ - specific reaction rate of target nuclide
R_N - specific reaction rate of radionuclide

Activation equation

Due to radioactive decay,
the number of radioactive nuclei
N decreases with time

$$N = \frac{N_1^0 \; R_{X,1}}{\lambda}(1 - e^{-\lambda t_{irr}})e^{-\lambda t}$$

The reaction rate of the radioactive nuclei *N*

$$\frac{dN}{dt} = -\lambda N$$

is proportional to the count rate measured by the detector.

The result is the **number of counts** in the full-energy peak (N_p) with the start of detection at time t_d after the end of irradiation:

$$N_p = \frac{N_1^0 \; R_{X,1}}{\lambda}(1 - e^{-\lambda t_{irr}})e^{-\lambda t_d}(1 - e^{-\lambda t_m})\,\gamma\,\varepsilon_p$$

$$\downarrow$$

$$\frac{N_p}{t_m} = N_1^0 \, R_{X,1}(1 - e^{-\lambda t_{irr}})\, e^{-\lambda t_d}\, \frac{(1 - e^{-\lambda t_m})}{\lambda t_m}\gamma\,\varepsilon_p$$

$$S = 1 - e^{-\lambda \, t_{irr}}$$

Factor for saturation during irradiation

$$D = e^{-\lambda \, t_d}$$

Decay factor

$$C = \frac{(1 - e^{-\lambda \, t_m})}{\lambda \; t_m}$$

“Measurement” factor

Activation equation

$$\frac{N_p}{t_m} = \frac{w N_A \Theta}{M} R_{X,1} \, S \, D \, C \, \gamma \, \varepsilon_p$$

ε_p Full-energy peak detection efficiency, including gamma attenuation

γ Probability of γ emission

Activity, *A* [s^{-1}] or the total count rate in the detector:

$$A = N_1^0 \, R_{X,1} \, \gamma \, \varepsilon_p = \frac{w N_A \Theta}{M} R_{X,1} \, \gamma \, \varepsilon_p$$

Specific count rate (s^{-1} g^{-1})

$$A_{sp} = \frac{N_A \Theta}{M} R_{X,1} \, \gamma \, \varepsilon_p$$

or

$$A_{sp} = \frac{N_p / t_m}{S \, D \, C \, w}$$

Activation equation

Specific count rate (s^{-1} g^{-1})

$$A_{sp} = \frac{N_A\ \Theta}{M} \frac{1}{F_{burn}} (G_{th}\, \varphi_{th}\, \sigma_0 + G_e\, \varphi_e\, I_0(\alpha))\ \gamma\ \varepsilon_p$$

Specific count rate under Cd activation (s^{-1} g^{-1})

$$(A_{sp})_{Cd} = \frac{N_A\ \Theta}{M} \frac{1}{F_{Cd}} G_e\ \varphi_e\, I_0(\alpha)\ \gamma\ \varepsilon_p$$

Nuclear research reactor
TRIGA Mark II (250 kW)

- Short and long irradiation in the CC:

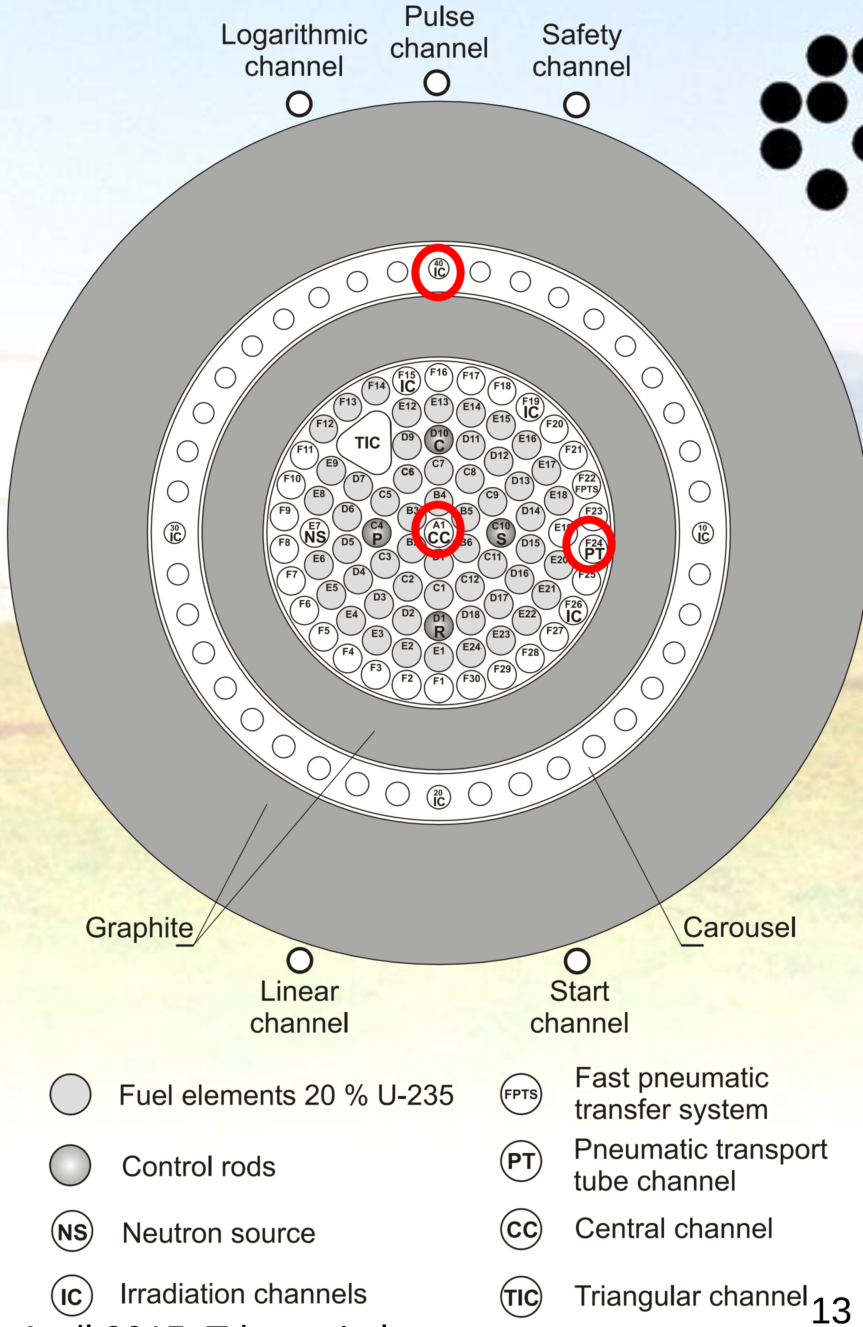
$\varphi_{th} \sim 10 \cdot 10^{12}\ cm^{-2}\ s^{-1}$

- Short irradiation in the PT and in the FPTS (up-to 30 min.)

$\varphi_{th} \sim 3.5 \cdot 10^{12}\ cm^{-2}\ s^{-1}$

- Long irradiation in the IC-40 (typically 20 hours)

$\varphi_{th} \sim 1.1 \cdot 10^{12}\ cm^{-2}\ s^{-1}$



Nuclear data of the target and nuclide formed

El.	Nuclide	$T_{1,2}$	$\sigma_{0,1}$, b	$I_{0,1}$, b	$\sigma_{0,N}$, b	$I_{0,N}$, b
Ru	^{105}Rh	35.36 h	0.32	4,3	16000	17000
Eu	^{152}Eu	13.516 y	5900	1510	12800	1580
Eu	^{152m}Eu	9.113 h	3304	1790	70000	1580
Gd	^{153}Gd	240.4 d	735	2020	36000	n. d.
Au	^{198}Au	2.695 d	98.65	1550	25100	31031
n. d.: no data						

Burn-up factor (F_{burn}) in irradiation channels of the TRIGA reactor (calculations)

IC-40: $\varphi_{th} \sim 1.0 \cdot 10^{12}$ cm^{-2}s^{-1}
PT: $\varphi_{th} \sim 3.5 \cdot 10^{12}$ cm^{-2}s^{-1}
CC: $\varphi_{th} \sim 10 \cdot 10^{12}$ cm^{-2}s^{-1}

El.	Nuclide	$T_{1,2}$	F_{burn} (20 h)		
			IC-40	PT	CC
Ru	^{105}Rh	35.36 h	0.999	0.998	0.994
Eu	^{152}Eu	13.516 y	0.999	0.998	0.993
Eu	^{152m}Eu	9.113 h	0.998	0.993	**0.980**
Gd	^{153}Gd	240.4 d	0.999	0.995	0.987
Au	^{198}Au	2.695 d	0.999	0.997	**0.991**

El.	Nuclide	F_{burn} in the CC channel					
		1 h	**10 h**	**20 h**	**50 h**	**100 h**	**200 h**
Ru	^{105}Rh	1.000	0.997	0.994	0.988	0.980	0.973
Eu	^{152}Eu	1.000	0.997	0.993	0.983	0.967	0.935
Eu	^{152m}Eu	0.999	0.988	0.980	0.966	0.958	0.946
Gd	^{153}Gd	0.999	0.993	0.987	0.968	0.937	0.879
Au	^{198}Au	1.000	0.995	0.991	0.978	0.961	0.938

(n, γ) Activation Analysis: Principles of standardization

The mass of the element:

$$w_a = \frac{M_a}{N_A \Theta_a \gamma_a} \frac{\left(\frac{N_p / t_m}{S\,D\,C}\right)_a}{(G_{th,a}\varphi_{th,a}\sigma_{0,a} + G_{e,a}\varphi_{e,a} I_{0,a}(\alpha))\varepsilon_{p,a}}$$

Relative standardization:

$$w_a = \frac{\left(\frac{N_p / t_m}{D\,C}\right)_a}{\left(\frac{N_p / t_m}{D\,C\,w}\right)_s} \frac{G_{th,s} f + G_{e,s} Q_{0,s}(\alpha)}{G_{th,a} f + G_{e,a} Q_{0,a}(\alpha)} \frac{\varepsilon_{p,s}}{\varepsilon_{p,a}}$$

Concentration in relative standardization:

$$\rho_a = \frac{\left(\frac{N_p / t_m}{D\,C\,w}\right)_a}{\left(\frac{N_p / t_m}{D\,C\,w}\right)_s}$$

(n, γ) Activation Analysis: Principles of standardization

Single-comparator standardization: use of k-factors (experimentally determined)

$$k_c(s) = \frac{A_{sp,s}}{A_{sp,c}}$$

$$k_c(s) = \frac{M_c\ \Theta_s\ \gamma_s\ \sigma_{0,s}}{M_s\ \Theta_c\ \gamma_c\ \sigma_{0,c}}\ \frac{G_{th,s}\ f + G_{e,s}\ Q_{0,s}(\alpha)}{G_{th,c}\ f + G_{e,c}\ Q_{0,c}(\alpha)}\ \frac{\varepsilon_{p,s}}{\varepsilon_{p,c}}$$

$$\rho_a = \frac{\left(\frac{N_p / t_m}{S\,D\,C\,w}\right)_a}{\left(\frac{N_p / t_m}{S\,D\,C\,w}\right)_c} \cdot \frac{1}{k_c(s)}$$

(n, γ) Activation Analysis: Principles of standardization

Absolute (parametric) standardization:

$$\rho_a = \frac{\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_a}{\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_m} \frac{M_a\ \Theta_m\ \gamma_m\,\sigma_{0,m}}{M_m\ \Theta_a\ \gamma_a\,\sigma_{0,a}} \frac{G_{th,m}\ f + G_{e,m}\,Q_{0,m}(\alpha)}{G_{th,a}\ f + G_{e,a}\,Q_{0,c}(\alpha)} \frac{\varepsilon_{p,m}}{\varepsilon_{p,a}}$$

a - analyte
m – flux monitor
Condition that $\boldsymbol{\varphi_{th}}$, **f** and **α** remain constant during irradiation
Parameters M, Θ, γ, σ_0 for both taken from literature (accurate known !)

k_0-standardization: KAYZERO/SOLCOI

Thermal and epithermal activation:

$$\rho_a = \frac{\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_a}{\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_{Au}} \frac{1}{k_{0,Au}(a)} \frac{G_{th,Au}\, f + G_{e,Au}\, Q_{0,Au}(\alpha)}{G_{th,a}\, f + G_{e,a}\, Q_{0,a}(\alpha)} \frac{\varepsilon_{p,Au}}{\varepsilon_{p,a}}$$

Only epithermal activation:

$$\rho_a = \frac{\left[\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_{Cd}\right]_a}{\left[\left(\dfrac{N_p / t_m}{S\,D\,C\,w}\right)_{Cd}\right]_{Au}} \frac{1}{k_{0,Au}(a)} \frac{F_{Cd,Au}\, G_{e,Au}\, Q_{0,Au}(\alpha)}{F_{Cd,a}\, G_{e,a}\, Q_{0,a}(\alpha)} \frac{\varepsilon_{p,Au}}{\varepsilon_{p,a}}$$

k_0-standardization

$$k_{0,Au}(a) = \frac{M_{Au}\,\Theta_a\,\gamma_a\,\sigma_{0,a}}{M_a\,\Theta_{Au}\,\gamma_{Au}\,\sigma_{0,Au}}$$

Compound nuclear constant

Tabulated constant:

k_0, Q_0, $\bar{E}_r$

(experimentally measured)

$$Q_0(\alpha) = \frac{Q_0 - 0.429}{\left(\bar{E}_r\right)^{\alpha}} + \frac{0.429}{(2\alpha+1)(0.55)^{\alpha}}$$

Q_0-factor:

$Q_0 = I_0/\sigma_0$

$\sigma_{0,Au}$	98.65 ± 0.09 b (±0.09%)
$I_{0,Au}$	1550 ± 28 b (±1.8%)
θ_{Au}	100%
$Q_{0,Au}$	15.71 ± 0.28 b (±1.8%)

α	Epithermal fluence rate deviation from 1/E
$\bar{E}_r$	Effective resonance energy

k_0-library info:

http://www.kayzero.com/k0naa/k0naa/News/News.html

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The 2012 recommended k_0 database

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Abstract Many overview papers have been published with recommended nuclear data for use in the k_0 method of NAA and made available in scientific journals or in the form of a downloadable database. In September 2009, the k_0-International Scientific Committee formed the k_0-Nuclear Data Committee (k_0-NDC) whose first task was to collect all these data at a single place to facilitate updating and to correct any evident errors. This task of the k_0-NDC was successfully completed in March 2012 when the 2012 recommended k_0 database was published in the form of an Excel file.

Keywords k_0 method of NAA · k_0 database · Nuclear data · The IUPAC k_0 database

[1], whereby absolute nuclear data were replaced by k_0 factors, which were experimentally determined. Compared to the relative method, the k_0 method greatly reduces the need for the preparation of standards. It uses gold as the standard and composite nuclear constants for analytically interesting nuclides are normalised to gold nuclear data. During the last 30 years the k_0 method has been introduced in many laboratories around the world for multi-element NAA and the method is continuously improving, along with its nuclear data [2–7]. In 2003, these data were made available by the International Union of Pure and Applied Chemistry (IUPAC) in the form of the Access database (http://www.iupac.org/home/projects/project-db/project-details.html?tx_wfqbe_pi1%5Bproject_nr%5D=2001-075-1-500) created by Kolotov and De Corte [8, 9]. In the process of validation of the consistency of the

k_0-library info:

http://www.kayzero.com/k0naa/k0naa/News/News.html

- The k_0-Nuclear Data Committee (k_0-NDC) is responsible for reviewing all new developments in the nuclear data used with the k_0 method of NAA, which includes ensuring the consistency in the k_0 database.
- The latter task was successfully fulfilled in March 2012 when the 2012 recommended k_0 database was published in the form of an Excel file dated 2012-03-14.

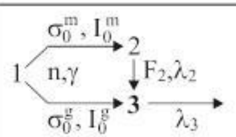
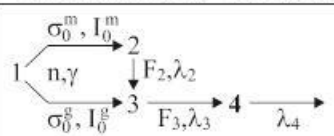
Periodic table of the elements (elements in the k_0-library)

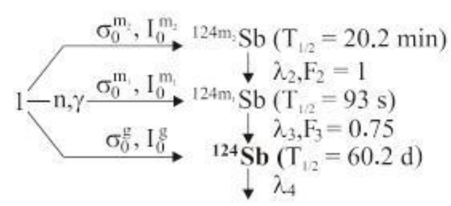
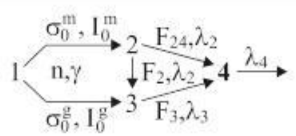
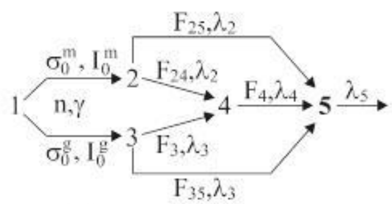
IA	IIA	IIIB	IVB	VB	VIB	VIB	{	VIII	}	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 *La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 □Ac															

*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
□	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Short irradiation (1-5 min) **Long irradiation (15 - 20 hours)**

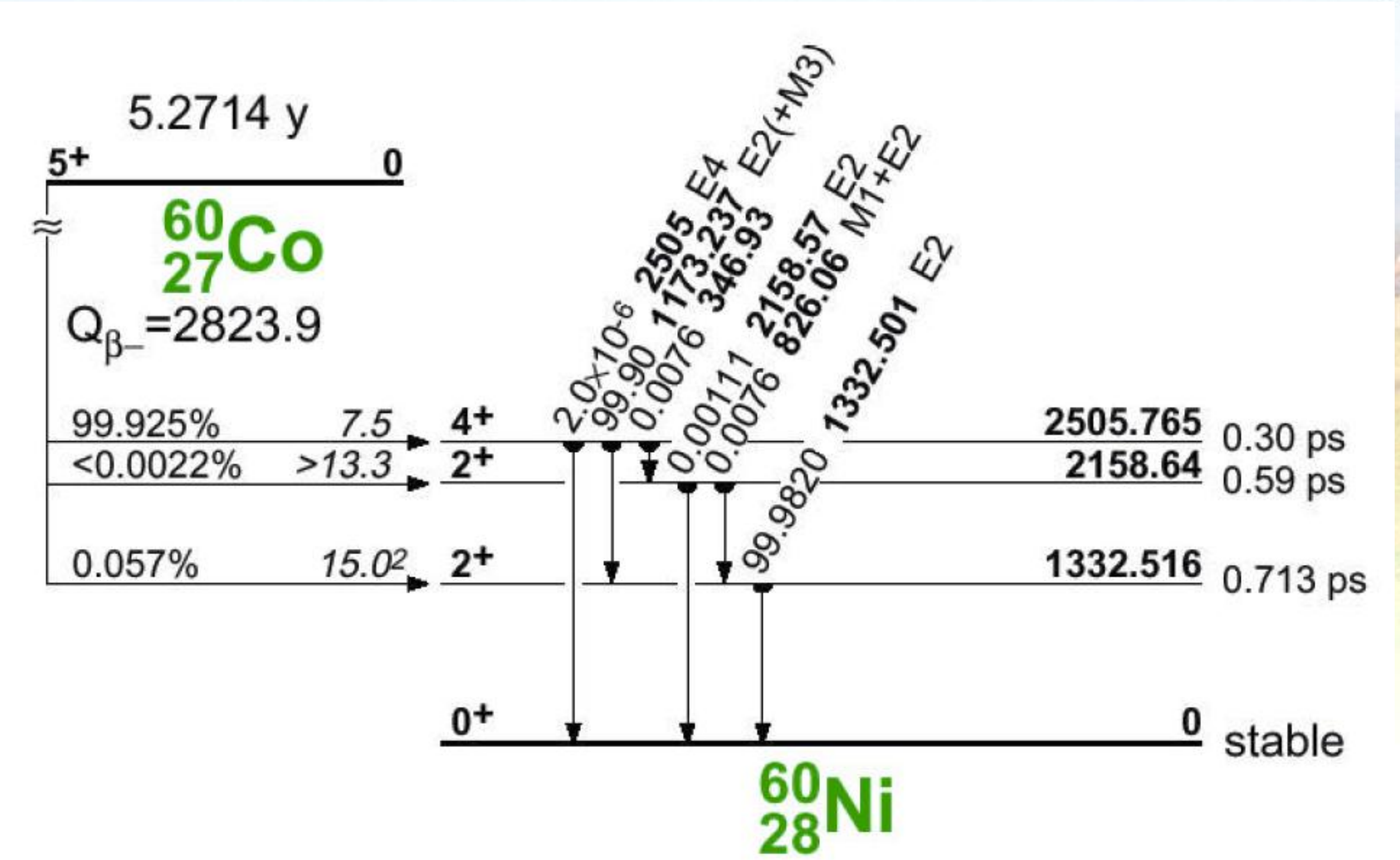
○ Westcott factor g ≠ 1

Type	Activation-decay scheme
I	$1 \xrightarrow[\sigma_0,\, I_0]{n,\gamma} \mathbf{2} \xrightarrow{\lambda_2}$ [e.g. ^{75}As (n, γ) ^{76}**As**]
IIa	$1 \xrightarrow[\sigma_0,\, I_0]{n,\gamma} 2 \xrightarrow{F_2,\lambda_2} \mathbf{3} \xrightarrow{\lambda_3}$ [e.g. ^{101}**Tc** from ^{100}Mo (n, γ)]
IIb	Special case: $\lambda_2 >> \lambda_3$ and $D_2 = 0$ [e.g. ^{233}**Pa** from ^{232}Th (n, γ)]
IIc	Special case: $\lambda_2 < \lambda_3$ and $D_3 = 0$
IId	Special case: measurement of the 140.5 keV line of ^{99}Mo /^{99m}Tc [from ^{98}Mo (n, γ)]
IIIa	$1 \xrightarrow[\sigma_0,\, I_0]{n,\gamma} 2 \xrightarrow{F_2,\lambda_2} 3 \xrightarrow{F_3,\lambda_3} \mathbf{4} \xrightarrow{\lambda_4}$; $2 \xrightarrow{F_{24},\lambda_2} \mathbf{4}$ [e.g. ^{97}**Nb** from ^{96}Zr (n, γ)]
IIIb	Special case: $F_{24} = 0$
IIIc	Special case: $\lambda_3 >> \lambda_2$ and λ_4, $D_3 = 0$ $F_3 = 1$, $F_2 + F_{24} = 1$ [e.g. ^{105}**Rh** from ^{104}Ru (n, γ)]
IVa	 [e.g. ^{80}**Br** from ^{79}Br (n, γ)]
IVb	Special case: $\lambda_2 >> \lambda_3$ and $D_2 = 0$ [e.g. ^{60}**Co** from ^{59}Co (n, γ)]
IVc	Special case: $\lambda_2 < \lambda_3$ and $D_3 = 0$
Va	

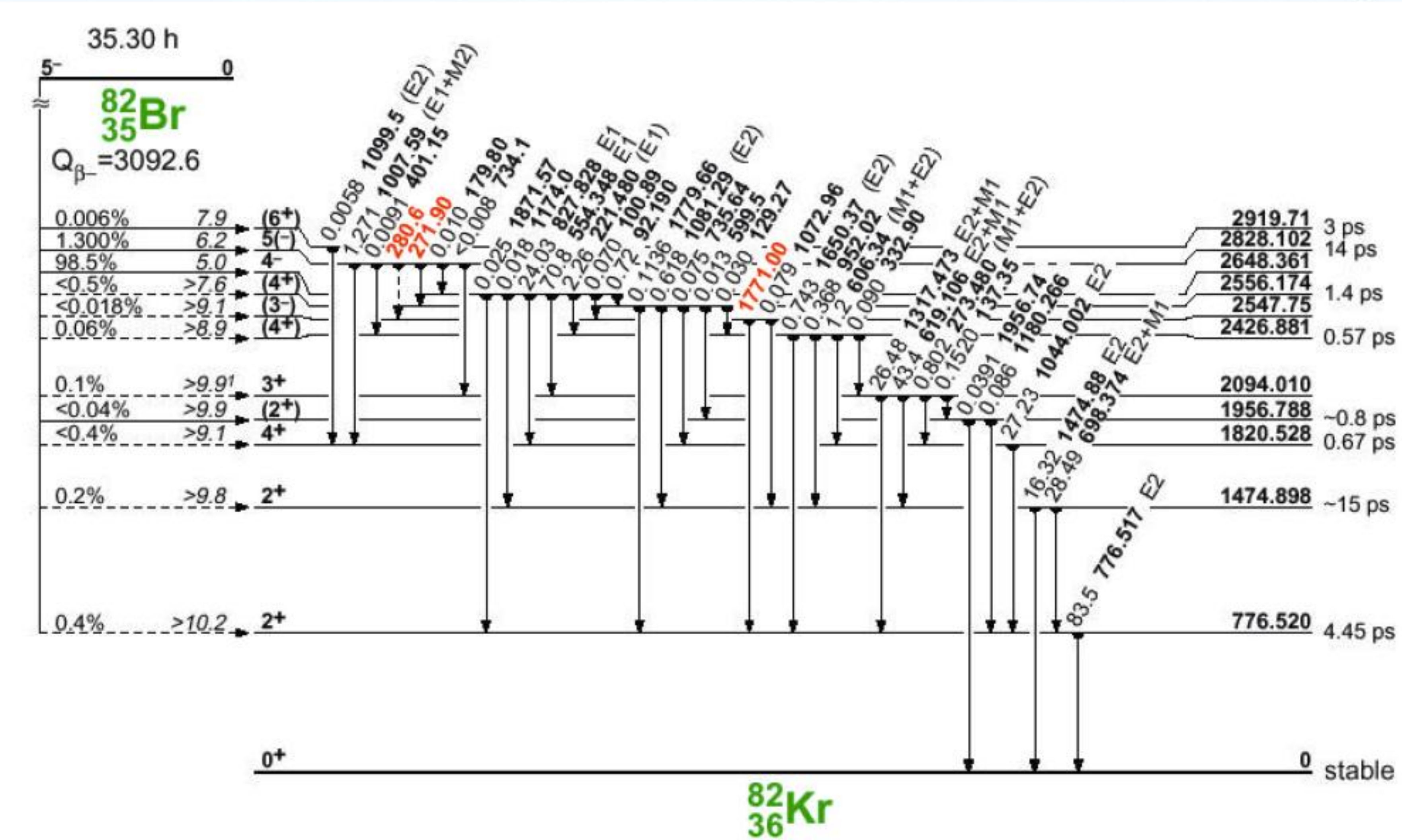
Type	Activation-decay scheme
Vb	Special case: $\lambda_4 << \lambda_2$ and λ_3 [e.g. ^{199}**Au** from ^{198}Au (n, γ)]
Vc	Special case: $\lambda_3 << \lambda_2$ and λ_4, $D_2 = D_4 = 0$ [e.g. ^{113m}**In** from ^{112}Sn (n, γ)]
VI	Special case: ^{124}**Sb** [from ^{123}Sb (n, γ)] after long decay time $(D_2 = D_3 = 0)$ 
VIIa	
VIIb	Special case: $F_2 = 0$ [e.g. ^{125}**Sb** from ^{124}Sn (n, γ)]
VIII	 [e.g. ^{117}**In** from ^{116}Cd (n, γ)]

Activation and decay types in the k_0-method

Decay scheme of the radionuclide



Decay scheme of the radionuclide



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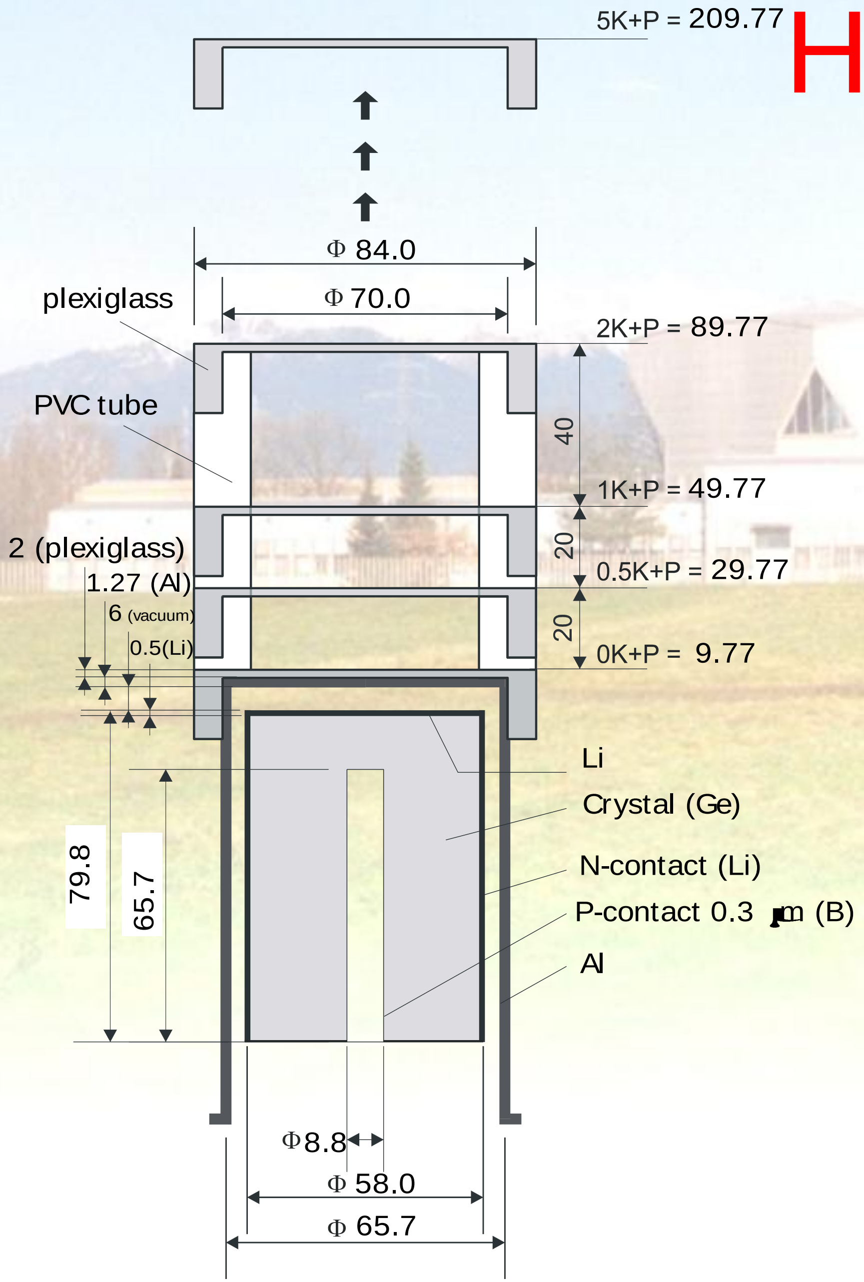
HPGe detector



HPGe closed end coaxial detector (OR4)
40% relative efficiency at 1332.5 keV (^{60}Co)
("fine tuning" dimensions are in mm)

Full-energy peak detection efficiency

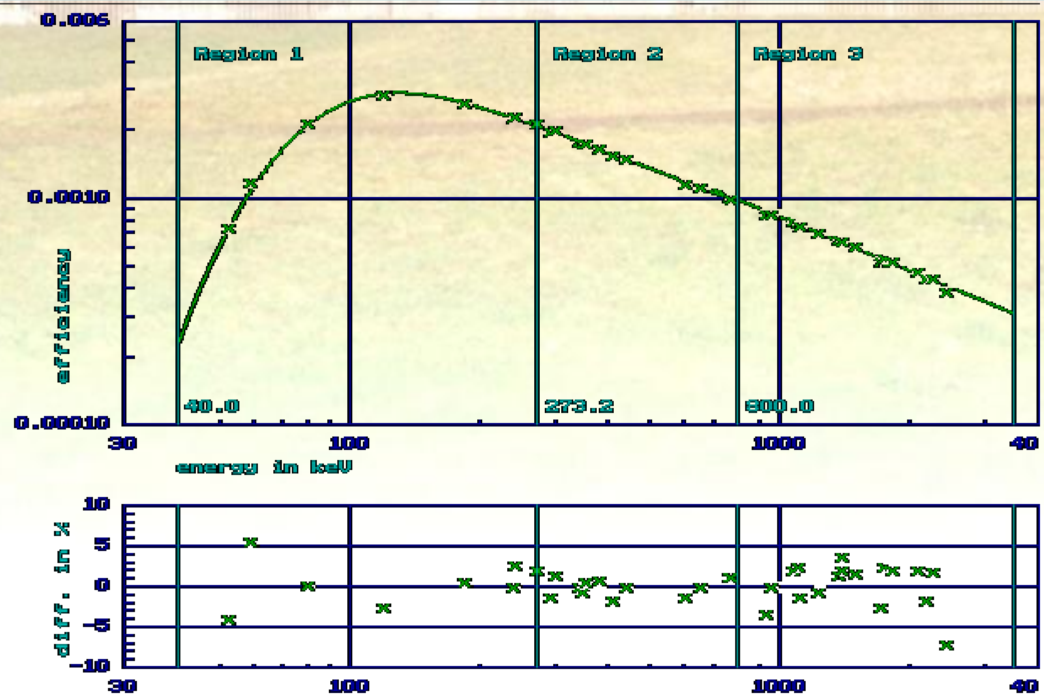
$$\varepsilon_{p,x} = \varepsilon_{p,ref} \frac{\bar{\Omega}_x}{\bar{\Omega}_{ref}}$$

Point sources at reference distance (20 cm):

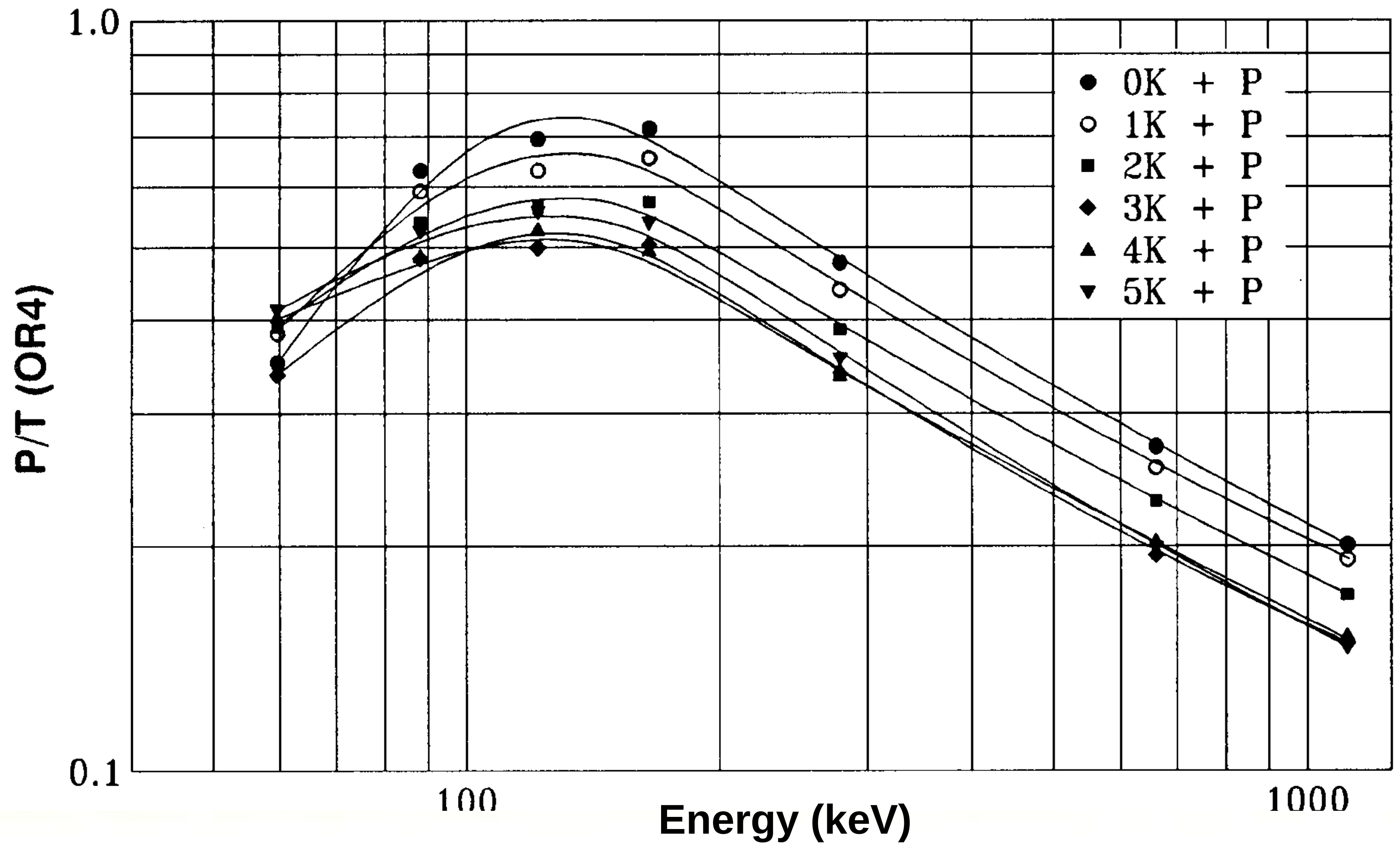
Am-241, Ba-133, Bi-207, Cd-109, Co-57, Co-60, Cr-51, Cs-137, Eu-152, Mn-54, Na-24, Ra-226, Sr-85

Fitting curve:

$$\log \varepsilon_p = a_0 + a_1(\log E_\gamma) + a_2(\log E_\gamma)^2 + a_3(\log E_\gamma)^3 + \ldots + a_n(\log E_\gamma)^n$$



Peak-to-total ratio (P/T)



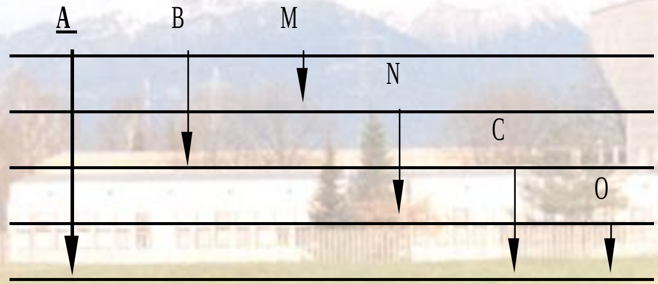
Coincidence free point sources:

Am-241, Cd-109, Co-57, Hg-203, Cr-51, Cs-137 and Zn-65

True coincidence correction factors

True coincidence effects occur when two or more cascading radiations give rise to a total or partial energy deposition in the HPGe detector

1. γ-γ coincidence summing



$$S(\underline{A}=B+C)=\frac{\gamma_B}{\gamma_A}a_C\,c_C\,\frac{\varepsilon_{p,B}\,\varepsilon_{p,C}}{\varepsilon_{p,A}}$$

γ - absolute gamma-intensity,

a – branching ratio,

$c = 1/(1+\alpha_t)$, α_t = total internal conversion coefficient ($= \alpha_K + \alpha_L + \ldots$),

ε_p – full-energy peak efficiency

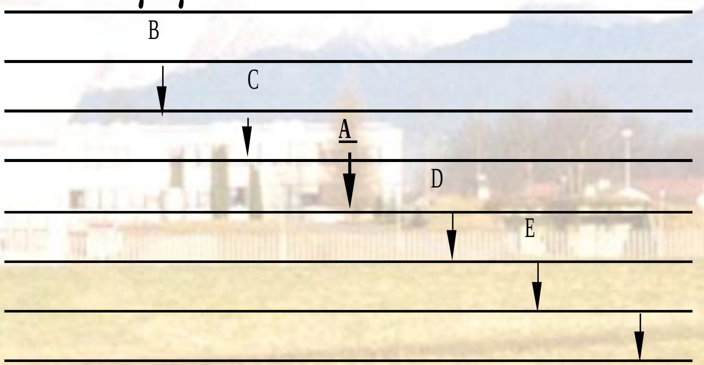
3. γ-KX(IC) Coincidence loss

4. γ-KX(EC) Coincidence loss

5. γ-511 keV (β^+) Coincidence loss

6. 511 keV(β^+)-511 keV(β^+) Coincidence loss

2. γ-γ coincidence loss



$$L(\underline{A}-D)=a_D\,c_D\,\varepsilon_{t,D}$$

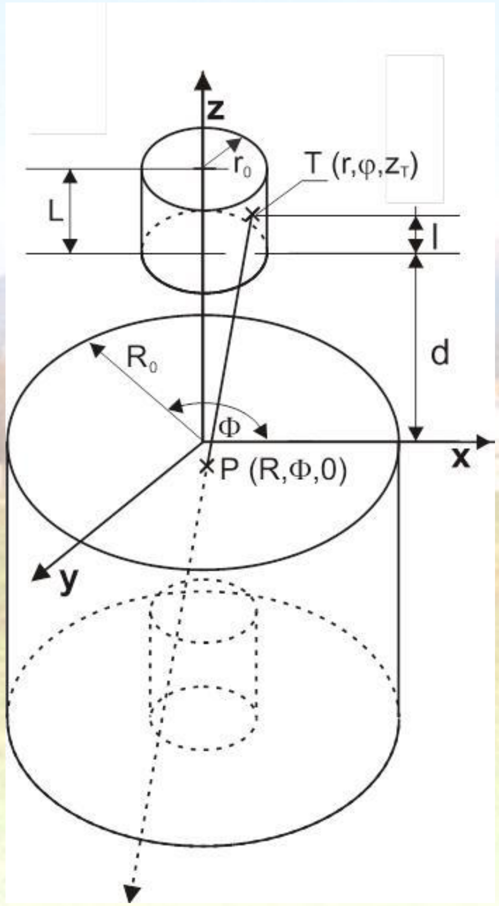
$$\varepsilon_{t,D}=\frac{\varepsilon_{p,D}}{P/T}$$

Total efficiency

$$COI = [1-L(\underline{A})]\cdot[1+S(\underline{A})]$$

$$N_{p,A}=\frac{N^*_{p,A}}{COI}$$

Effective solid angle



$$F_{att} = e^{\left(-\sum_{i=1}^{m} \mu_i \delta_i\right)}$$

Gamma attenuation caused by incoherent interaction in the absorbing material interposed between source and detector body

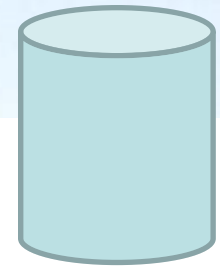
$$F_{eff} = f_1 + f_2 f'$$

Probability for a photon with E_γ to interact incoherently with the detector material

$$\bar{\Omega} = \frac{4}{r_0^2 L} \int_0^L (d+l)dl \int_0^{r_0} rdr \int_0^{\pi} d\Phi \int_0^{R_0} \frac{F_{att} F_{eff} RdR}{[R^2 - 2Rr\cos\Phi + r^2 + (d+l)^2]^{3/2}}$$

COI factors for OR4 detector

ϕ=8 mm
h=5 mm



ρ =1 g cm^{-3}

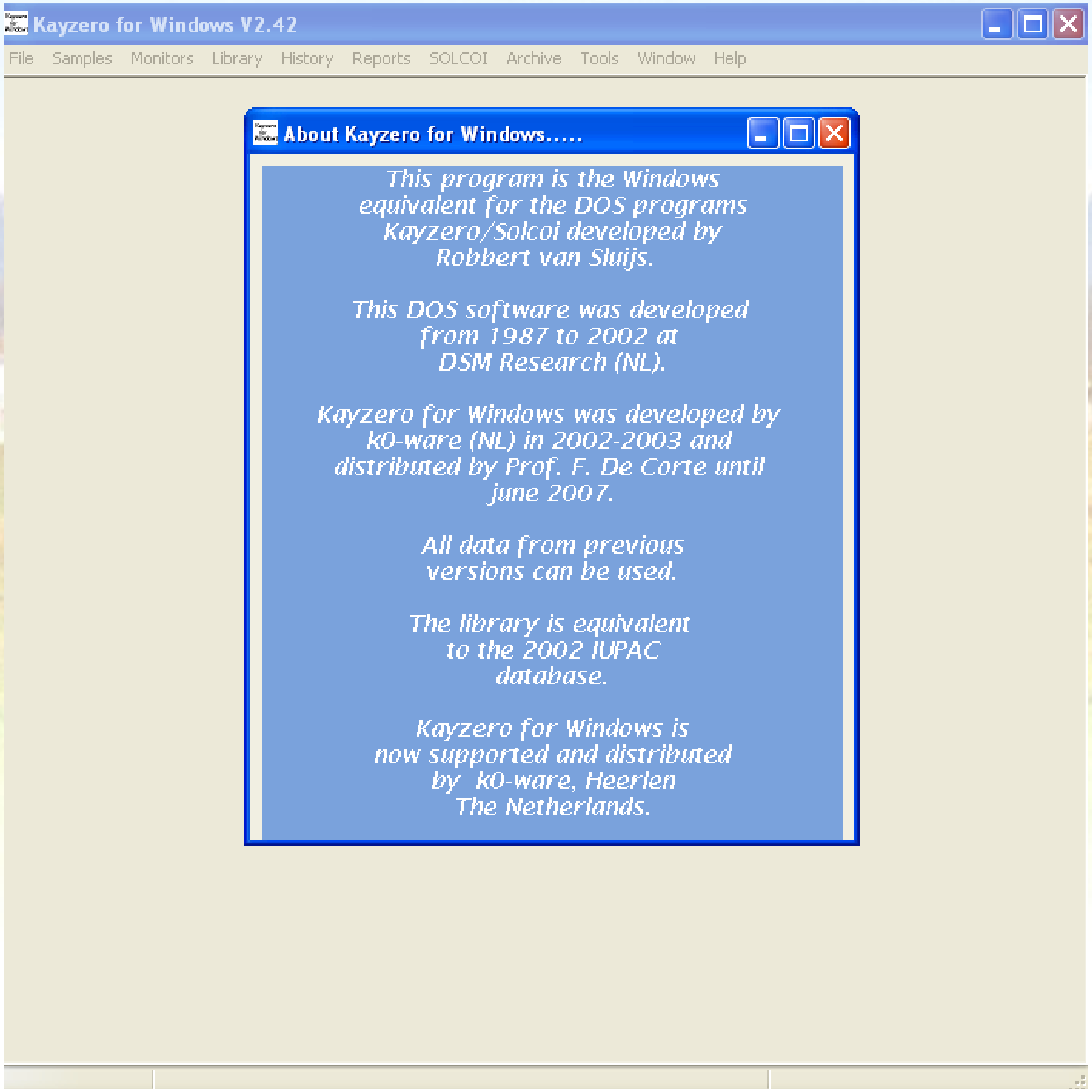
```
Volume monsterhouder =     .25701  cm3
Aantalposities        = 5
Coincidentiefactoren voor SPRONK AAA 0905 SEDIMENT
Detector or4
Pulse shaping time =  4.000 microsec.
Matrix materiaal = #CaCO3
Aantal isotopen in het bestand :   139
```

	1 cm	3 cm	5 cm	7 cm	21 cm
CO60 2					
1173.2 keV	.84229	.93254	.96304	.97584	.99504
1332.5 keV	.83850	.93095	.96219	.97530	.99499
BR82 16					
92.2 keV	.71242	.86605	.92468	.95029	.98996
221.3 keV	.71846	.86725	.92514	.95056	.99013
273.5 keV	.56291	.79297	.88315	.92282	.98467
554.3 keV	.64272	.83524	.90777	.93928	.98791
606.3 keV	.55354	.78808	.88086	.92162	.98496
619.1 keV	.61022	.81808	.89786	.93270	.98674
698.4 keV	.56301	.79293	.88329	.92303	.98497
776.5 keV	.64971	.83883	.90991	.94074	.98831
827.8 keV	.69618	.86372	.92427	.95021	.99001
952.0 keV	.59131	.80856	.89297	.92980	.98672
1007.5 keV	.69403	.86261	.92369	.94987	.98996
1044.0 keV	.67435	.85256	.91804	.94621	.98942
1081.3 keV	.59743	.81057	.89593	.93322	.98811
1317.5 keV	.74287	.88845	.93841	.95911	.99168
1474.8 keV	.77573	.90533	.94805	.96526	.99281
1650.3 keV	.75036	.89536	.94329	.96242	.99268

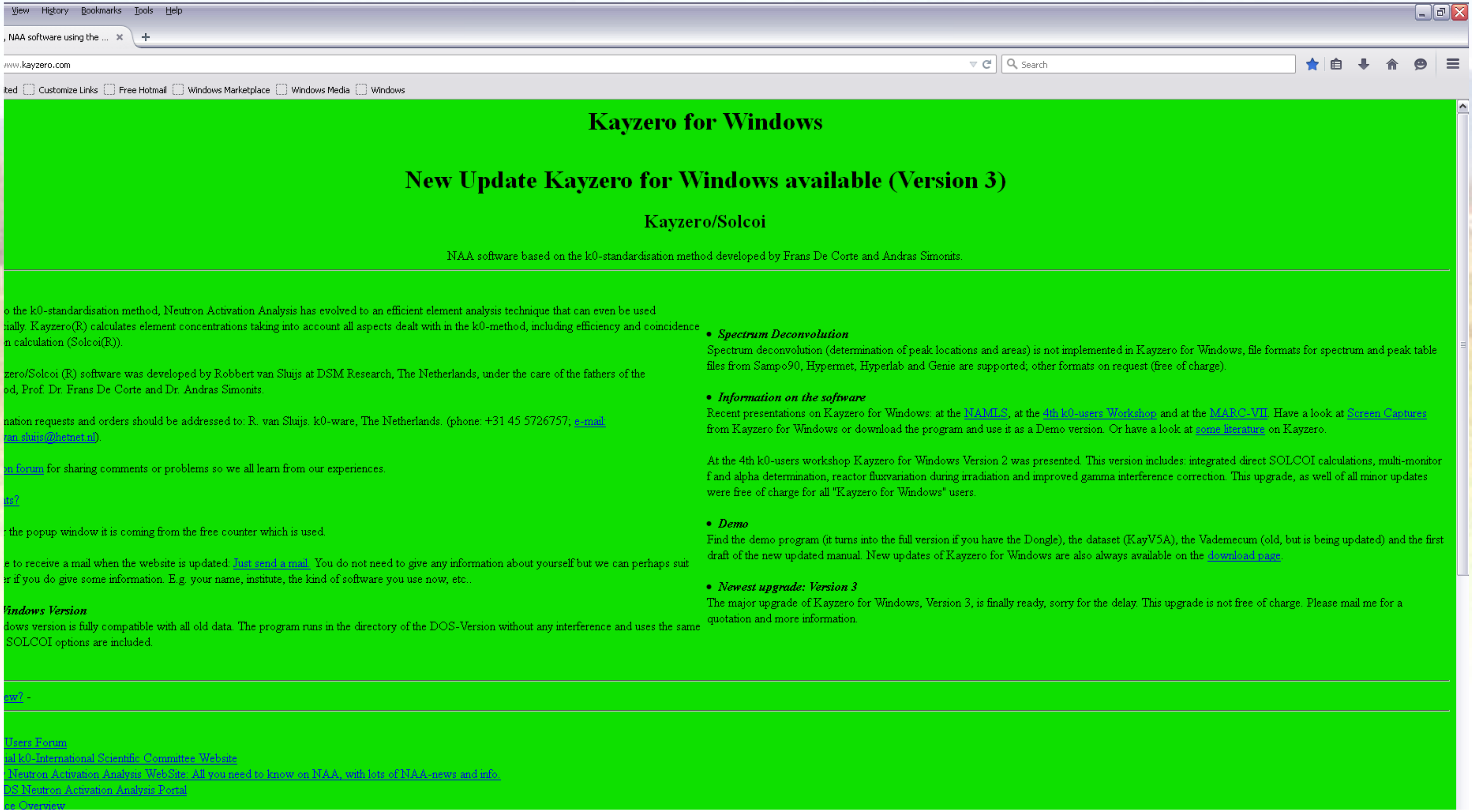
k_0-standardization: KAYZERO/SOLCOI

- k_0-standardization method of NAA was launched in the 1970s
- **SINGCOMP** program: 1987 written for VAX
- **KAYZERO/SOLCOI** program: 1994, 1996, 2003 written for **DOS** and in 2004 written for **Windows**
- Current status: Kayzero for Windows (**KayWin®**) ver. 2.42 from March 2011
- KAYZERO library - 144 nuclides (68 elements)
- k_0-NAA became widespread as a practical analytical tool used to analyse different sample matrices

KAYZERO/SOLCOI (KayWin) software



KayWin: http://www.kayzero.com/


View History Bookmarks Tools Help
, NAA software using the ...
www.kayzero.com
ited Customize Links Free Hotmail Windows Marketplace Windows Media Windows

Kayzero for Windows

New Update Kayzero for Windows available (Version 3)

Kayzero/Solcoi

NAA software based on the k0-standardisation method developed by Frans De Corte and Andras Simonits.

o the k0-standardisation method, Neutron Activation Analysis has evolved to an efficient element analysis technique that can even be used
ially. Kayzero(R) calculates element concentrations taking into account all aspects dealt with in the k0-method, including efficiency and coincidence
n calculation (Solcoi(R)).

zero/Solcoi (R) software was developed by Robbert van Sluijs at DSM Research, The Netherlands, under the care of the fathers of the
od, Prof. Dr. Frans De Corte and Dr. Andras Simonits.

nation requests and orders should be addressed to: R. van Sluijs. k0-ware, The Netherlands. (phone: +31 45 5726757; e-mail:
van.sluijs@hetnet.nl).

on forum for sharing comments or problems so we all learn from our experiences.

its?

the popup window it is coming from the free counter which is used.

e to receive a mail when the website is updated: Just send a mail. You do not need to give any information about yourself but we can perhaps suit
r if you do give some information. E.g. your name, institute, the kind of software you use now, etc..

Vindows Version
dows version is fully compatible with all old data. The program runs in the directory of the DOS-Version without any interference and uses the same
SOLCOI options are included.

- ***Spectrum Deconvolution***
Spectrum deconvolution (determination of peak locations and areas) is not implemented in Kayzero for Windows, file formats for spectrum and peak table files from Sampo90, Hypermet, Hyperlab and Genie are supported; other formats on request (free of charge).

- ***Information on the software***
Recent presentations on Kayzero for Windows: at the NAMLS, at the 4th k0-users Workshop and at the MARC-VII. Have a look at Screen Captures from Kayzero for Windows or download the program and use it as a Demo version. Or have a look at some literature on Kayzero.

At the 4th k0-users workshop Kayzero for Windows Version 2 was presented. This version includes: integrated direct SOLCOI calculations, multi-monitor f and alpha determination, reactor fluxvariation during irradiation and improved gamma interference correction. This upgrade, as well of all minor updates were free of charge for all "Kayzero for Windows" users.

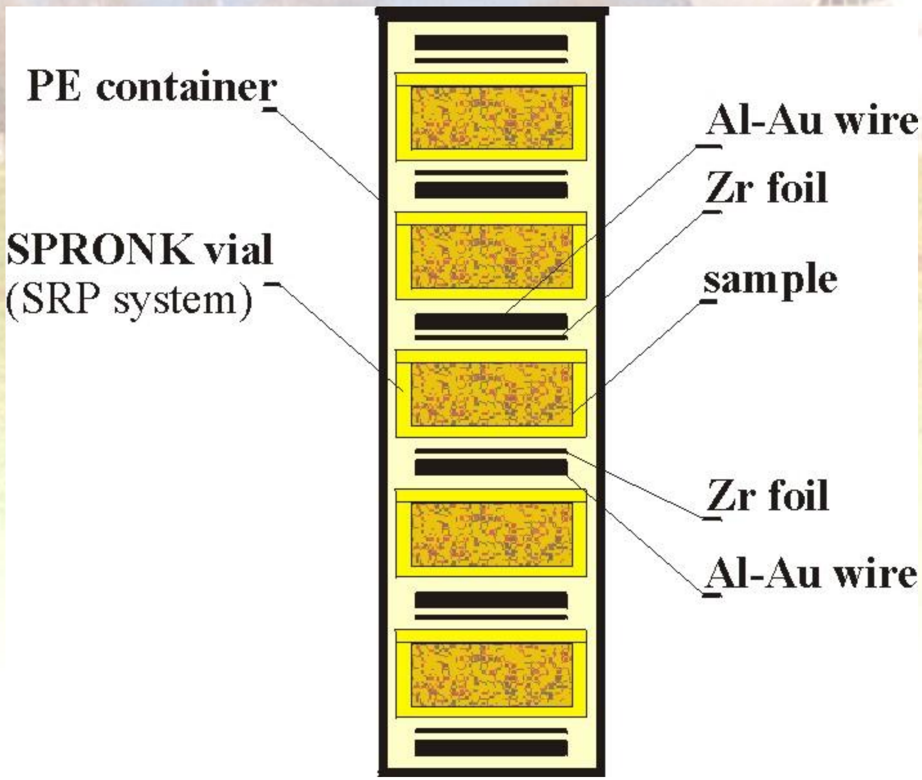
- ***Demo***
Find the demo program (it turns into the full version if you have the Dongle), the dataset (KayV5A), the Vademecum (old, but is being updated) and the first draft of the new updated manual. New updates of Kayzero for Windows are also always available on the download page.

- ***Newest upgrade: Version 3***
The major upgrade of Kayzero for Windows, Version 3, is finally ready, sorry for the delay. This upgrade is not free of charge. Please mail me for a quotation and more information.

ew? -

Users Forum
ial k0-International Scientific Committee Website
Neutron Activation Analysis WebSite: All you need to know on NAA, with lots of NAA-news and info.
DS Neutron Activation Analysis Portal
ce Overview

k_0-INAA analytical procedure



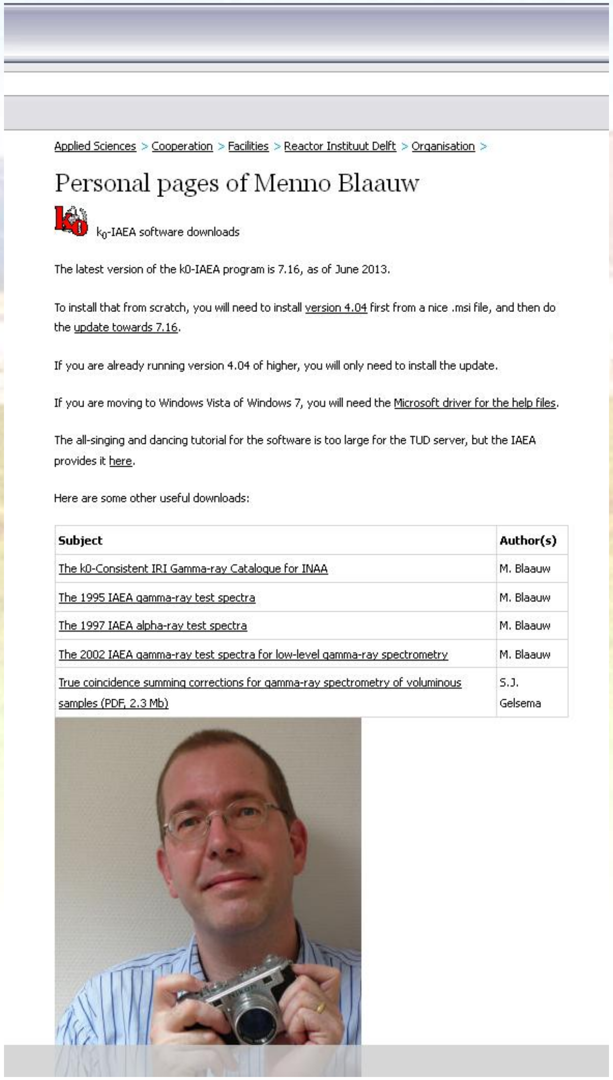
- Sample and standard are prepared in sandwich form and irradiated in the carousel facility of the TRIGA Mark II reactor (250 kW)
- Measurement on an HPGe absolutely calibrated detector
- Evaluation of the spectrum by HyperLab program
- Calculation of the effective solid angle between sample and HPGe detector
- Calculation of element concentration by KayWin®

k_0-IAEA software

- A new **k0_IAEA** software for k_0-NAA appeared in **2004** in collaborations between the **IAEA** (M. Rossbach), **M. Blaauw**, **M. Bacchi**, beta testers (L. Xilei, R. Jaćimović, G. Kenedy and M.C. Freitas) and additional programmer **A. Trkov**
- Current status: k0_IAEA software ver. 7.16 from June 2013
- From **ver. 4.01** of k0_IAEA software the Kayzero library has been updated. The new data have been obtained from:
  - [DECORTE2003]: Recommended nuclear data for use in the k0-standardization of neutron activation analysis, Atomic Data and Nuclear Data Tables **85 (2003) 47-67**
  - [DECORTE2003b]: The updated NAA nuclear data library derived from the Y2K k0-database, J. Radioanal. Nucl. Chem., **257 (2003) 493-499**
  - [IUPAC] Compilation of k0 and related data for NAA, V. P. Kolotov and F. De Corte, **ver. 4, 1.10.2002**

k_0-IAEA software

http://www.tnw.tudelft.nl/index.php?id=34350&L=1



CERTIFICATE OF ANALYSIS

SMELS

ASSIGNED VALUES [1]

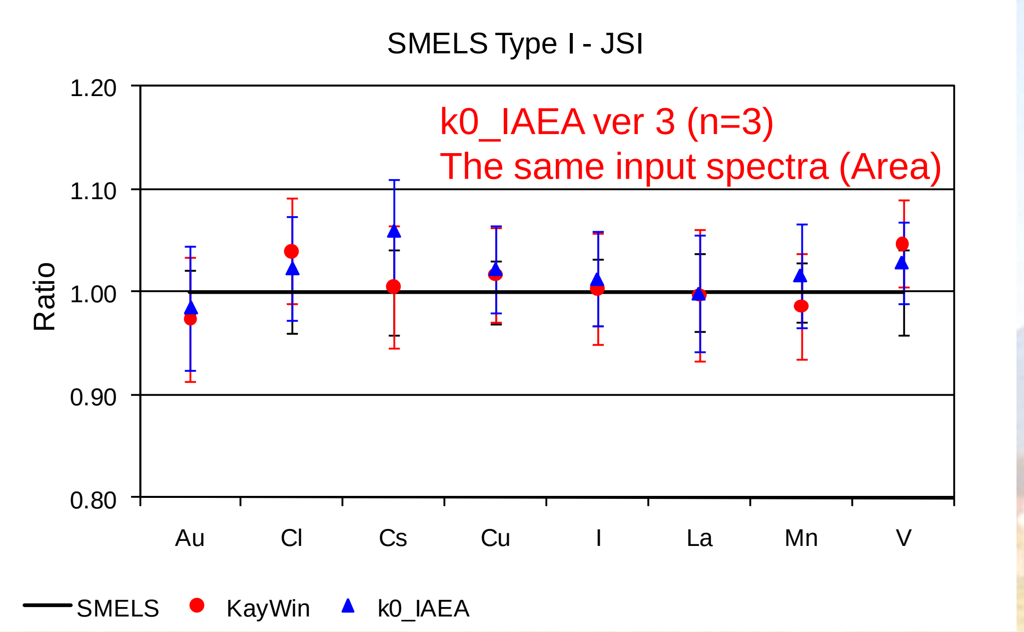
SMELS	Element	Assigned Value [1] ± U [2] [1] mg/kg	Number of withheld labs
Type I	Au	82,7 ± 1,7	8
	Cl	4330 ± 170	8
	Cs	897 ± 37	8
	Cu	3930 ± 120	8
	I	152 ± 5	7
	La	265 ± 10	8
	Mn	113,9 ± 3,3	8
	V	39 ± 1,6	8
Type II	As	92,3 ± 3,6	9
	Au	3,93 ± 0,07	9
	Br	157 ± 5	7
	Ce	15600 ± 800	7
	Mo	5170 ± 250	8
	Pr	1193 ± 37	8
	Sb	172 ± 8	9
	Th	3670 ± 180	9
	Yb	187 ± 10	9
	Zn	6570 ± 200	8
Type III	Au	0,901 ± 0,016	8
	Co	24,3 ± 0,33	9
	Cr	86,7 ± 2,6	9
	Cs	20,80 ± 0,34	8
	Fe	8200 ± 190	9
	In	462 ± 19	9
	Sb	51,2 ± 1,3	7
	Sc	1,140 ± 0,031	9
	Se	131 ± 6	9
	Sr	8150 ± 200	9
	Th	26,2 ± 0,9	9
	Tm	23,3 ± 0,7	7
	Yb	20,7 ± 0,5	9
	Zn	618 ± 11	9
	Zr	4580 ± 100	9

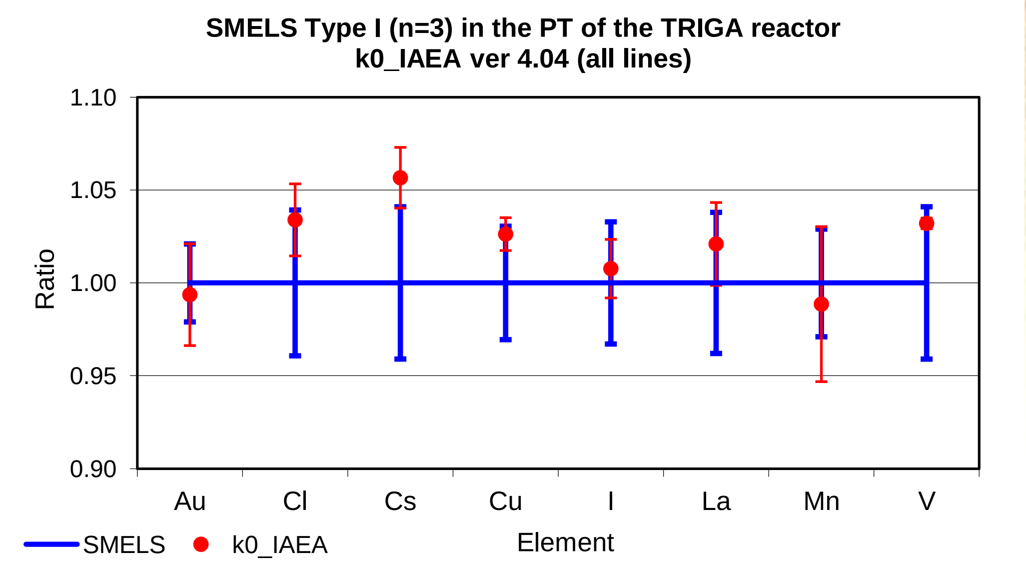
[1]: The assigned values, as determined after a characterisation exercise [1], represent total contents. These values are not traceable to SI and are not certified.
[2]: Estimated expanded uncertainty U with a coverage factor k=2, corresponding to a level of confidence of about 95 %, as defined in the Guide to the Expression of Uncertainty in Measurement (GUM), ISO, 1995. Uncertainty contributions arising from characterisation as well as from homogeneity and stability assessment were taken into consideration.

SMELS page 1 of 3

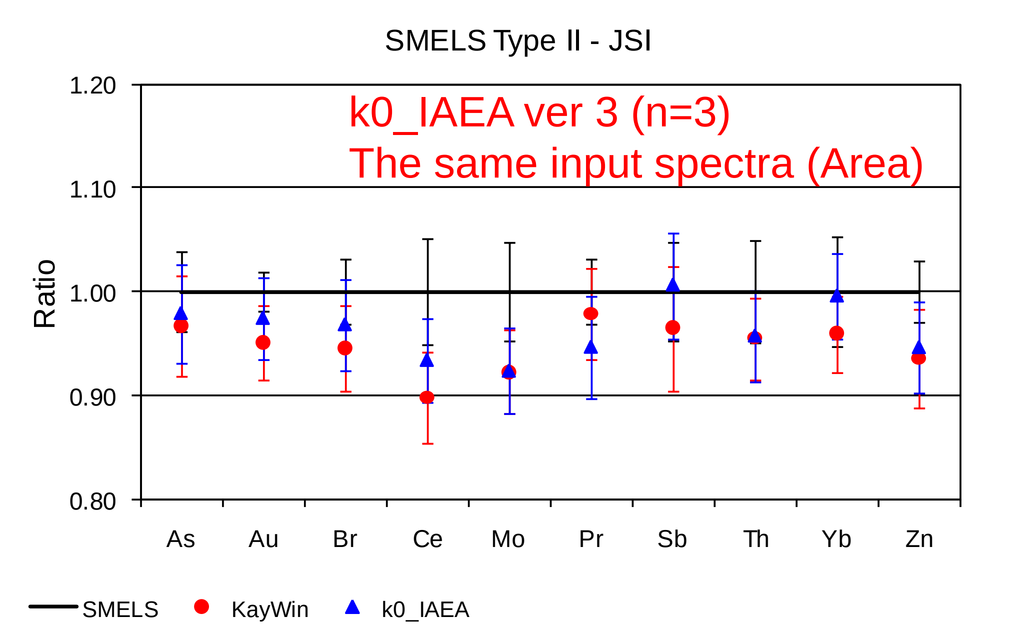
P. Vermaercke, et al., Nucl. Instr. Meth. A 564 (2006) 675-682

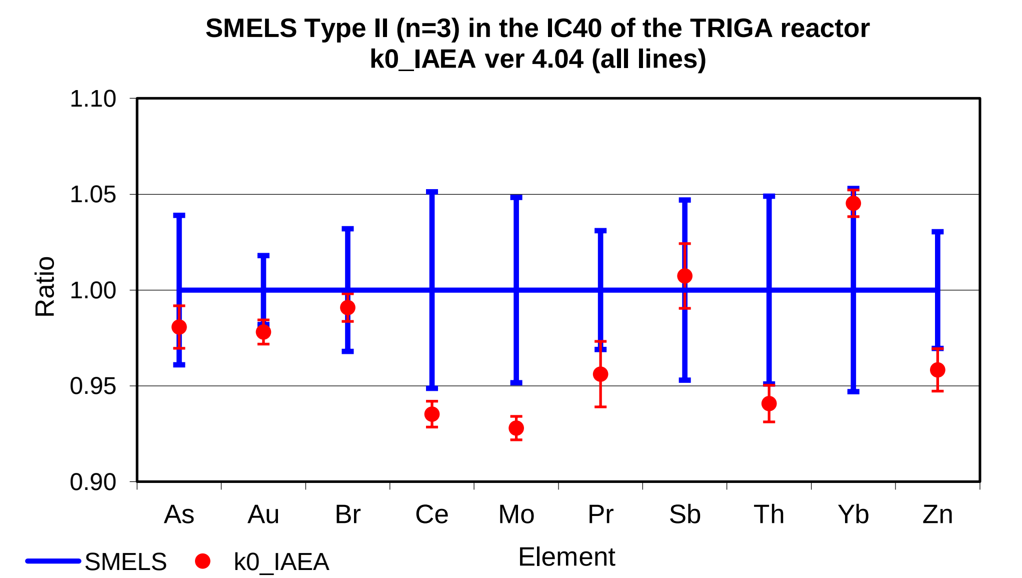
KayWin vs. k0_IAEA



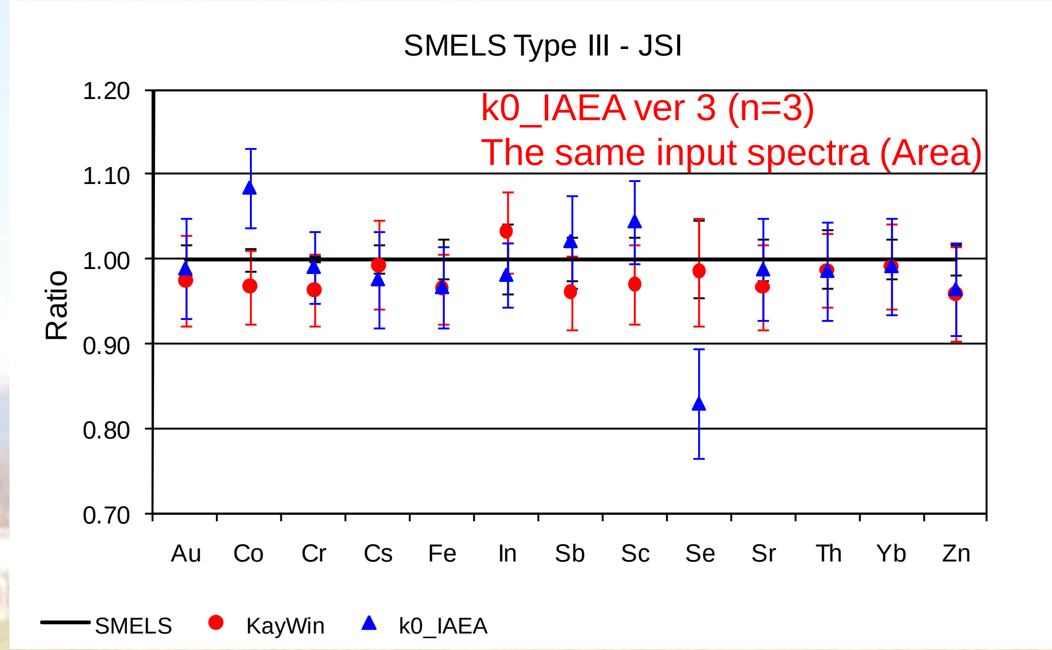


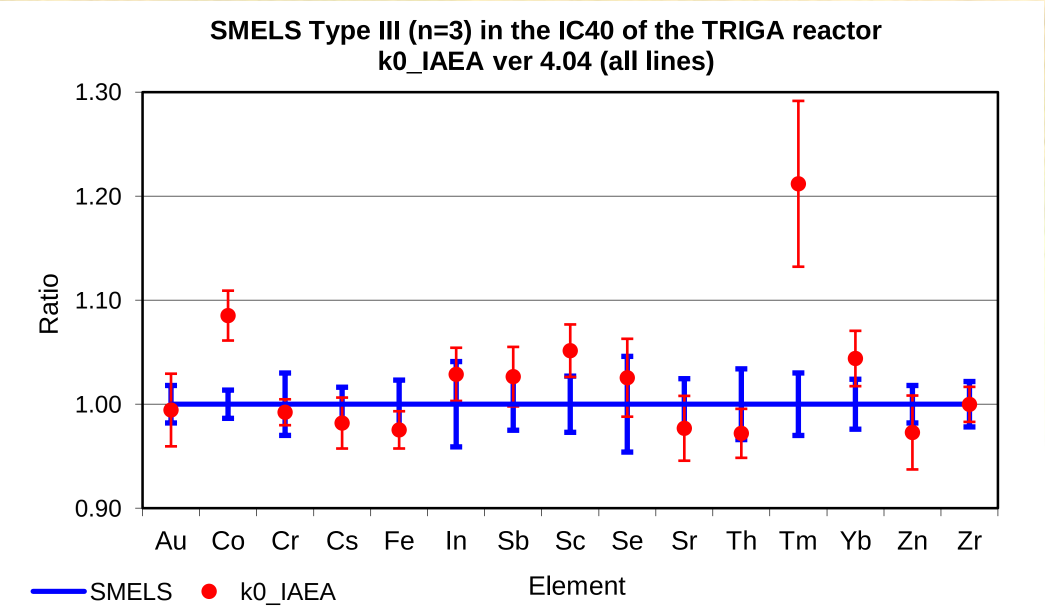
KayWin vs. k0_IAEA





KayWin vs. k0_IAEA





Acknowledgments

- The IAEA, Austria
- Prof. F. De Corte, Belgium
- Dr. A. Simonits, Hungary
- Robbert van Sluijs, The Netherlands
- Dr. Menno Blaauw, The Netherlands
- Colleagues at the Department of Environmental Sciences at the JSI, Slovenia

Practical exercise:

KayWin

and

k_0-IAEA software