2484-12

ICTP-IAEA Joint Workshop on Nuclear Data for Science and Technology: Medical Applications

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Compilation and standardization of data

TARKANYI Ferenc Tibor

Institute of Nuclear Research, Hungarian Academy of Sciences
Debrecen
Hungary

Compilation and standardization of data

- Applied nuclear data users seldom rely on numerical data extracted directly from original publications. Instead, they utilize evaluated (recommended) data. These are values distilled from consideration by experienced evaluators of the body of existing experimental and theoretical numerical results. Evaluators strive to produce the most reliable possible recommendations, based on critical assessments of the quality of data available from the reported scientific studies. This applies to both nuclear structure and nuclear reaction data (*e.g.*, reaction cross sections).
- In earlier times, the evaluation of nuclear reaction data often involved drawing smooth eye guides through plots of measured experimental data extracted from the literature. The "error" bars (uncertainties) shown in these plots inevitably influenced evaluators, but only subjectively. This approach is no longer viewed as acceptable. More sophisticated and objective data evaluation procedures have evolved during the last several decades. Weights are assigned to nuclear reaction data sets, according to their perceived quality. Judgments on quality are based on both the uncertainties quoted by authors and evaluator impressions as to the reliability of these estimates.
- It is important for experimenters to provide reasonable and well-documented uncertainty data for their reported results, regardless of which physical parameters are measured.

Nuclear Data Sheets 113 (2012) 3006–3053

Topics

- **Flow chart of measurement, processing and application of nuclear data**
- **Why not only model results?**
- **Nuclear data in nuclear medicine**
- **Nuclear data needs in medical applications**
- **Present work: nuclear reaction data for production of medical radioisotopes and CP beam monitoring**
- **The data evaluation process**
  - **Status of experimental database**
  - **Compilation of experimental data**
  - **Correction and selection of th experimental data**
  - **Fitting methods**
- **Development and status of the evaluated nuclear reaction database for production of diagnostic and therapeutic radioisotopes and charged particle monitor reactions**

Flow chart of measurement, processing and application of nuclear data

- **Data measurement**
- **Compilation**
- **Critical analysis**
- **Selection**
- **Model calculation**
- **Evaluation**
- **Application**

Nuclear reaction theory and model calculations

- **Application field (complementary to experiments)**
  - **Many CPND to evaluate**
  - **Very difficult to measure**
  - **Unpredictable time delay**
  - **Expensive, manpower**
- **A priory model calculations**
  - **To show the tendencies**
  - **To filter the controversial data**
  - **To make more realistic estimations**
  - **To make quick estimations**
  - ***Very limited accuracy, ”approximately*”**
- **Models with appropriate parameters based on experimental data**
- **The present power:**
  - **For extrapolation and interpolation of experimental data**
  - **To predict unknown nuclear data like cross section, angular and energy distribution, double differential cross sections**
  - **To check inconsistencies between measurements**

Nuclear data needs for medical applications

Field of application	Type of nuclear data		
	Decay	Reaction	Structure
Diagnostics			
SPECT	yes	yes	(th)
PET	yes	yes	(th)
Therapy			
endo	yes	yes	(th)
tele			
X	no	no	no
γ	yes	yes	(th)
e	yes	yes	(th)
p	yes	yes	(th)
n	yes	yes	(th)
HI	yes	yes	(th)
Others	yes	yes	(th)

Other medical related nuclear data needs

- Standard data for monitoring beam parameters
- Standard data for dosimetry
- Radiation safety

Present lecture

Cross section data related to medical isotope production:

production cross sections

production yields

CP monitor reactions

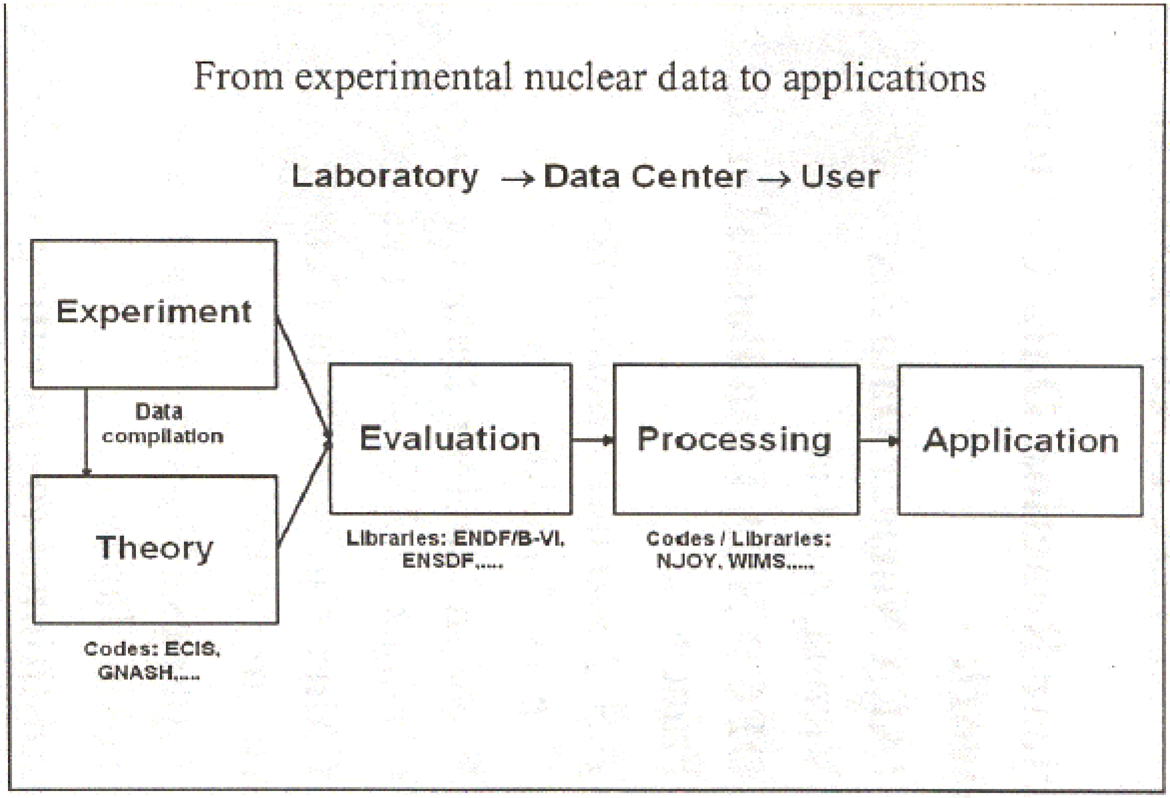
Radioisotope production

- **Nuclear reaction data in radioisotope production are needed mainly for optimization of production routes**
- **Selection of the optimal production route**
- **Selection of the projectile energy range**
- **Minimize the radioactive impurities**
- **Real practical importance:**
  - **Few hundred cyclotrons**
  - **Many nuclear reactors**

Data evaluation

- Before being used in applications, the experimental and theoretical data must pass through an evaluation stage.
- Detailed compilation and critical review of experimental and theoretical data to make the necessary corrections and to select the best data.
- Derivation of preferred values by appropriate combination of different processes (fitting, theory, systematics).
- Recommended data are generated in different ways dependent on the available experimental data, on the capability of the model codes, on the requested accuracy of the application.

Process of data evaluation



Definition of (ND) Evaluation

A properly weighted combination (usually by GLSQ fit) **of selected experimental data** (and nuclear reaction modeling results).

“Non-model”; GLSQ fit: standards

Model prior + GLSQ fit

R. Capote EFNUDAT Workshop, Paris

Overview of Nuclear Data Evaluation Methods

- **Selection of experimental data and EXFOR**
- **Experimental uncertainties and correlations**
- **Modeling uncertainties**

  Model defects

  Model parameters
- **GLSQ**
- **UMC formulation**
- **UMC+TMC**

R. Capote EFNUDAT Workshop, Paris

Main steps of the evaluation

- ***Evaluation of experimental data***
  - **Collection**
  - **Data analysis**
  - **Comparison**
  - **Correction**
  - **Analysis of existing model results and syst.**
  - **New measurements**
  - **Critical assessment and selection**
- ***Experimental data processing***
  - **Data fit**
  - **Legendre polynomials**
  - **Orthogonal polynomials**
  - **Spline functions**
  - **Rational functions**
  - **Fitted model results**
  - **Eye guide**
- ***Experiment based model calculations***
  - **Different models, different capabilities for different parameters for different energy ranges**
  - **Adjusted model input parameters to agree with experimental results**

Collection of experimental data

- **Scientist, specialist in the field!!!**
- **Collection**
  - **Full use of all available data**
  - **Importance of original publications**
  - **Database bibliography**
- **Data analysis**
  - **Method of measurements**
  - **Experimental technique**
  - **Error calculation**
  - **Nuclear data**
  - **Laboratory**
  - **Definitions**
  - **Purpose**
  - **Data evaluation**
- **Correction for misrepresentation of experimental technique**
- **Correction according to new standard data**
- **Comparison**
- **The data are plotted to compare with other experimental results**
- **Analysis of existing model results and systematics for orientation (threshold, magnitude, shape)**
- **New measurements - Dedicated, if necessary**

Critical analysis and selection

- **Necessary corrections, if the data are important and the correction is reasonable**
- **Single and simultaneous evaluation and selection process**
- **Equal weight selection or deselecting of minority data sets**
- **Normalization of systematically amplitude shifted data to fill the gaps**
- **Main problem: lack of information in the publications**

Experimental data processing

- **Data fit**
  - **Legendre polynomials**
  - **Orthogonal polynomials**
  - **Spline functions**
  - **Rational functions**
  - **Fitted model results (ALICE, GNASH,EMPIRE, TALYS)**
  - **Eye guide**

- **Problems**

- **Realistic uncertainties**
  - **Covariances**
  - **Scattered points**
  - **Not existing resonances**
  - **Existing resonances**
  - **Energy scale problems**

IAEA CRP for standardization of cross section databases for medical radioisotope production and beam monitoring

- **Charged Particle Cross-Section Database for Medical Radioisotope Production: Diagnostic Radioisotopes and Monitor Reactions (1996-2001) CRP-I**
- **IAEA-TECDOC-1211**

- **Nuclear Data for the Production of Therapeutic Radionuclides (2003-2007) CRP-II**
- **TECHNICAL REPORTS SERIES NO. 473 STI/DOC/010/473**

- **Nuclear Data for Charged-particle Monitor Reactions and Medical Isotope Production (2012-2016) CRP-III**

Charged Particle Cross-Section Database for Medical Radioisotope Production: Diagnostic Radioisotopes and Monitor Reactions (1996-2001) CRP-I

CRP-I Monitor Reactions

Protons	Deuterons	^{3}He-particles	Alpha-particles
$^{27}Al(p,x)^{22}Na$	$^{27}Al(d,x)^{22}Na$	$^{27}Al(^{3}He,x)^{22}Na$	$^{27}Al(\alpha,x)^{22}Na$
$^{27}Al(p,x)^{24}Na$	$^{27}Al(d,x)^{24}Na$	$^{2}7Al(^{3}He,x)^{24}Na$	$^{27}Al(\alpha,x)^{24}Na$
$^{nat}Ti(p,x)^{48}V$	$^{nat}Ti(d,x)^{48}V$	$^{nat}Ti(^{3}He,x)^{48}V$	$^{nat}Ti(\alpha,x)^{51}Cr$
$^{nat}Ni(p,x)^{57}Ni$	$^{nat}Fe(d,x)^{56}Co$		$^{na}tCu(\alpha,x)^{66}Ga$
$^{nat}Cu(p,x)^{56}Co$	$^{nat}Ni(d,x)^{61}Cu$		$^{nat}Cu(\alpha,x)^{67}Ga$
$^{nat}Cu(p,x)^{62}Zn$			$^{nat}Cu(\alpha,x)^{65}Zn$
$^{nat}Cu(p,x)^{63}Zn$			
$^{nat}Cu(p,x)^{65}Zn$			

CRP-I Gamma emitters

^{67}Ga

$^{67}Zn(p,n)^{67}Ga$

$^{68}Zn(p,2n)^{67}Ga$

^{123}I

$^{123}Te(p,n)^{123}I$

$^{124}Te(p,2n)^{123}I$

$^{124}Te(p,n)^{124}I$

^{81}Rb

$^{82}Kr(p,2n)^{81}Rb$

$^{nat}Kr(p,x)^{81}Rb$

^{201}Pb

$^{203}Tl(p,3n)^{201}Pb$

$^{203}Tl(p,2n)^{202m}Pb$

$^{203}Tl(p,4n)^{200}Pb$

^{111}In

$^{111}Cd(p,n)^{111}In$

$^{112}Cd(p,2n)^{111}In$

^{123}Xe

$^{127}I(p,5n)^{123}Xe$

$^{127}I(p,3n)^{125}Xe$

^{123}Cs

$^{124}Xe(p,2n)^{123}Cs$

$^{124}Xe(p,pn)^{123}Xe$

CRP-I- Positron emitters

^{11}C

$^{14}N(p,\alpha)^{11}C$

^{13}N

$^{16}O(p,\alpha)^{13}N$

^{15}O

$^{15}N(p,n)^{15}O$

$^{14}N(d,n)^{15}O$

^{18}F

$^{18}O(p,n)^{18}F$

$^{nat}Ne(d,x)^{18}F$

^{68}Ge

$^{69}Ga(p,2n)^{68}Ge$

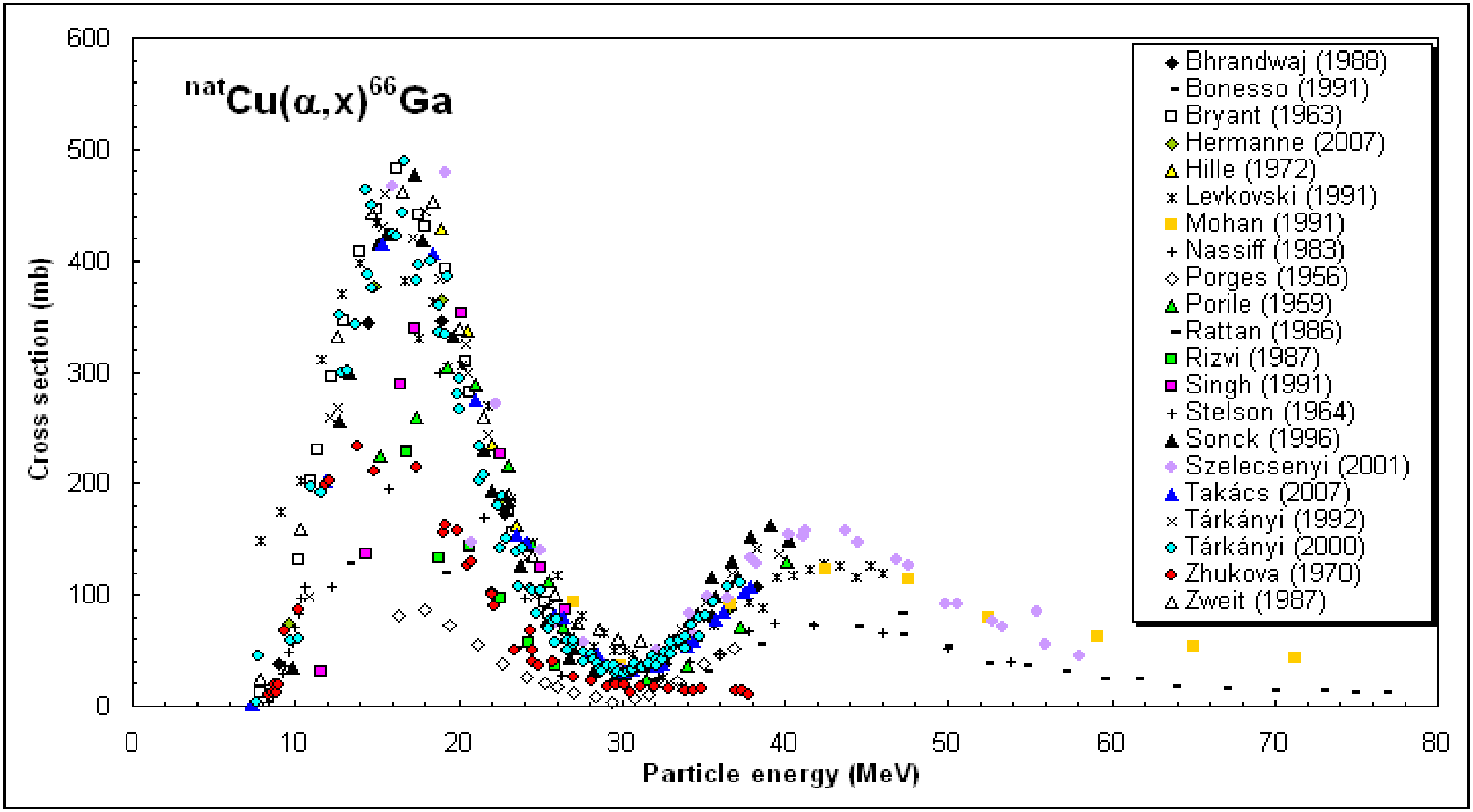
$^{nat}Ga(p,x)^{68}Ge$

^{82}Sr

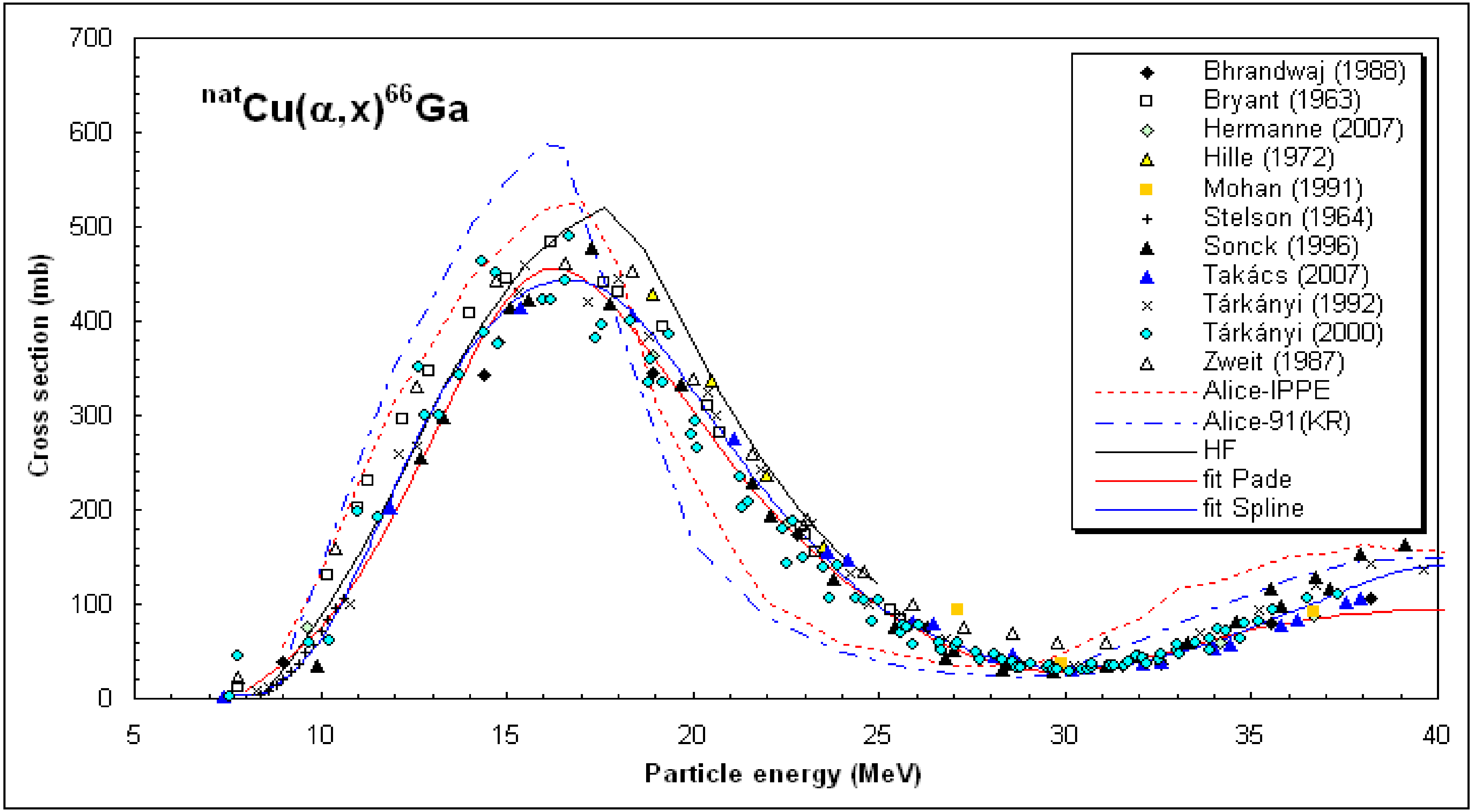
$^{85}Rb(p,4n)^{82}Sr$

$^{nat}Rb(p,x)^{82}Sr$

Typical example (all data)



Selected data and fitted curves



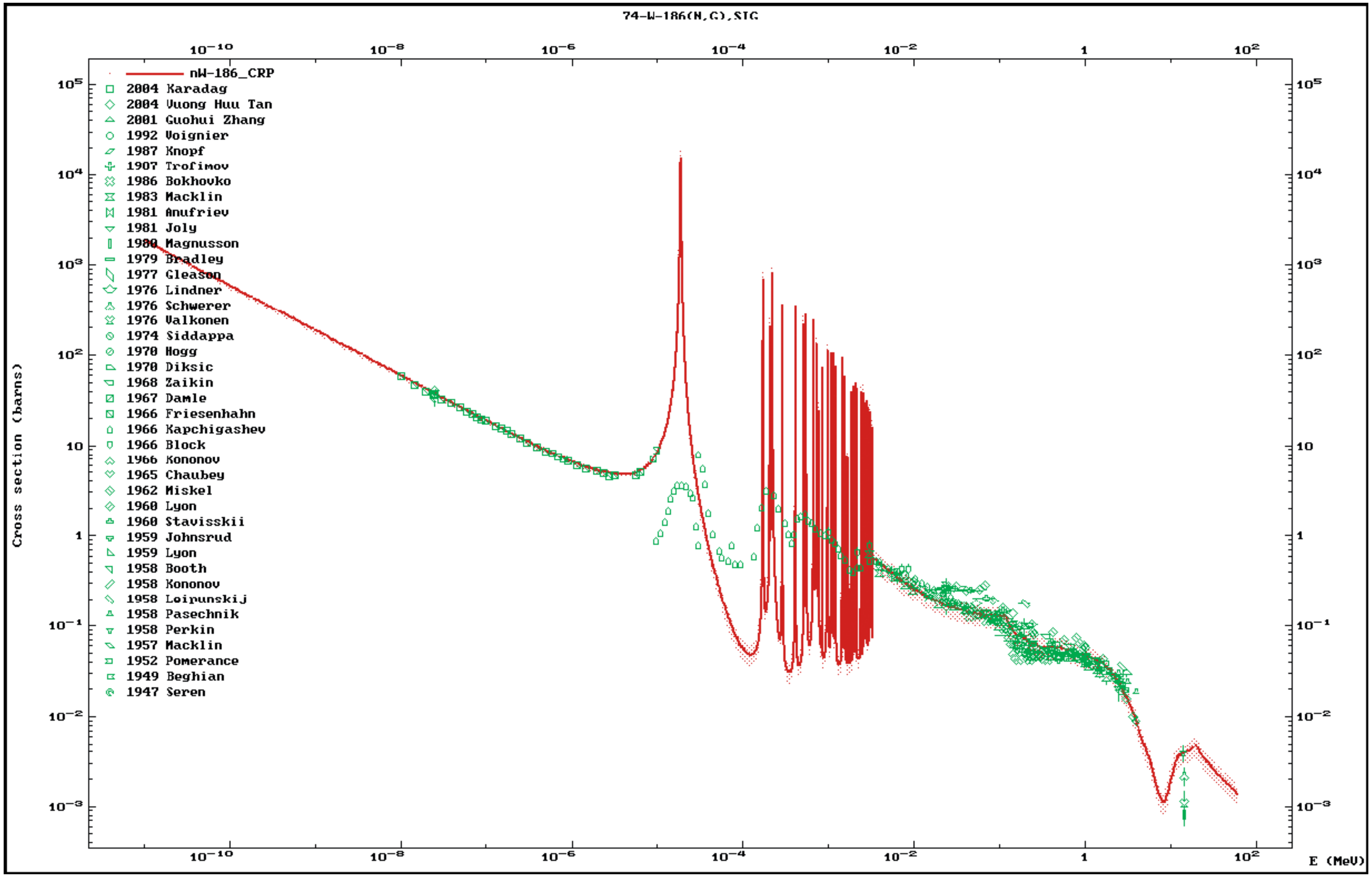
Nuclear Data for the Production of Therapeutic Radionuclides

CRP-II

CRP-II Production by reactors

- **Evaluation of fission yields for production of ^{90}Y, ^{131}I and ^{137}Cs radionuclides.**
- **Nuclear data for the production of ^{64}Cu, ^{114m}In, ^{166}Ho, ^{169}Yb, ^{177}Lu, ^{186}Re and ^{188}Re radionuclides through capture channels and decay.**
- **Nuclear data for the production of ^{32}P, ^{64}Cu, ^{67}Cu, ^{89}Sr, ^{90}Y and ^{153}Sm radionuclides through the charge-exchange (n, p) channel.**

Example ^{186}W neutron capture cross-section.



CRP-II Production by accelerators-I

^{103}Pd

^{103}Rh(p,n)^{103}Pd

^{103}Rh(p,pn)^{102}Rh

^{103}Rh(d,2n)^{103}Pd

^{103}Rh(d,p2n)^{102}Rh

^{186}Re

^{186}W(p,n)^{186}Re

^{186}W(d,2n)^{186}Re

^{192}Ir

^{192}Os(p,n)^{192}Ir

^{192}Os(d,2n)^{192}Ir

CRP-II Production by accelerators-II

^{64}Cu

^{64}Ni(p,n)^{64}Cu
^{64}Ni(d,2n)^{64}Cu
^{68}Zn(p,x)^{64}Cu
^{nat}Zn(d,x)^{64}Cu

^{67}Cu

^{68}Zn(p,2p)^{67}Cu
^{70}Zn(p,α)^{67}Cu

^{67}Ga

^{67}Zn(p,n)^{67}Ga
^{68}Zn(p,2n)^{67}Ga

^{86}Y

^{86}Sr(p,n)^{86}Y

^{111}In

^{111}Cd(p,n)^{111}In
^{112}Cd(p,2n)^{111}In

^{114m}In

^{114}Cd(p,n)^{114m}In
^{114}Cd(p,2n)^{114m}In
^{116}Cd(p,3n)^{114m}In

^{124}I

^{124}Te(p,n)^{124}I
^{125}Te(p,2n)^{124}I
^{124}Te(d,2n)^{124}I

^{125}I

^{125}Te(p,n)^{125}I
^{124}Te(d,n)^{125}I

^{169}Yb

^{169}Tm(p,n)^{169}Yb
^{169}Tm(d,2n)^{169}Yb

^{177}Lu

^{176}Yb(d,n)^{177g}Lu
^{176}Yb(d,p)^{177}Yb
^{176}Yb(d,x)^{177g}Lu

^{211}At

^{209}Bi(α,2n)^{211}At
^{209}Bi(α,3n)^{210}At

^{225}Ac

^{226}Ra(p,2n)^{225}Ac

Nuclear Data for Charged-particle Monitor Reactions and Medical Isotope

CRP-III

CRP-III Monitor reaction

Protons	**Deuterons**	**^{3}He-particles**	**Alpha-particles**
$^{27}Al(p,x)^{22}Na$	$^{27}Al(d,x)^{22}Na$	$^{27}Al(^{3}He,x)^{22}Na$	$^{27}Al(\alpha,x)^{22}Na$
$^{27}Al(p,x)^{24}Na$	$^{27}Al(d,x)^{24}Na$	$^{2}7Al(^{3}He,x)^{24}Na$	$^{27}Al(\alpha,x)^{24}Na$
$^{nat}Ti(p,x)^{48}V$	$^{nat}Ti(d,x)^{48}V$	$^{nat}Ti(^{3}He,x)^{48}V$	$^{nat}Ti(\alpha,x)^{51}Cr$
$^{nat}Cu(p,x)^{56}Co$	$^{nat}Ni(d,x)^{61}Cu$		$^{nat}Cu(\alpha,x)^{67}Ga$
$^{nat}Cu(p,x)^{62}Zn$	**$^{nat}Ti(d,x)^{46}Sc$**		$^{nat}Cu(\alpha,x)^{65}Zn$
$^{nat}Cu(p,x)^{63}Zn$	**$^{nat}Ni(d,x)^{56,58}Co$**		
$^{nat}Cu(p,x)^{65}Zn$	**$^{nat}Cu(d,x)^{62,63,65}Zn$**		
$^{nat}Mo(p,x)^{96g+m}Tc$			

CRP-III- Gamma Emitters

^{67}Ga

- ^{67}Zn(p,n)^{67}Ga
- ^{68}Zn(p,2n)^{67}Ga

^{123}I

- ^{123}Te(p,n)^{123}I
- ^{124}Te(p,2n)^{123}I
- ^{124}Te(p,n)^{12}4I

^{81}Rb

- ^{82}Kr(p,2n)^{81}Rb
- ^{nat}Kr(p,x)^{81}Rb

^{201}Pb

- ^{203}Tl(p,3n)^{201}Pb
- ^{20}3Tl(p,2n)^{202m}Pb
- ^{203}Tl(p,4n)^{200}Pb

^{111}In

- ^{111}Cd(p,n)^{111}In
- ^{112}Cd(p,2n)^{111}In

^{123}Xe

- ^{127}I(p,5n)^{123}Xe
- ^{12}7I(p,3n)^{125}Xe

^{123}Cs

- ^{124}Xe(p,2n)^{123}Cs
- ^{124}Xe(p,pn)^{123}Xe
- **^{124}Xe(p,x)^{121}I**

^{99}Mo

- **^{100}Mo(n,2n)^{99}Mo**
- **^{100}Mo(p,pn)^{99}Mo**
- **^{100}Mo(d,p2n)^{99}Mo**
- **^{100}Mo(γ,n)^{99}Mo**
- **^{238}U(γ,f)^{99}Mo**

^{99m}Tc

- ^{100}Mo(p,2n)$^{99g+m}$Tc
- ^{100}Mo(d,3n)$^{99g+m}$Tc

^{51}Cr

- ^{nat}Fe(p,x)^{51}Cr
- ^{51}V(p,n)^{51}Cr
- ^{51}V(d,2n)^{51}Cr
- ^{nat}Ti(α,x)^{51}Cr

CRP-III Positron emitters-I

^{11}C	^{13}N	^{15}O	^{18}F
$^{14}N(p,\alpha)^{11}C$	$^{16}O(p,\alpha)^{13}N$	$^{15}N(p,n)^{1}5O$	$^{18}O(p,n)^{18}F$
		$^{14}N(d,n)^{15}O$	$^{nat}Ne(d,x)^{18}F$

$^{68}Ge/^{68}Ga$	^{82}Sr	^{52}Fe	^{55}Co
$^{69}Ga(p,2n)^{68}Ge$	$^{85}Rb(p,4n)^{82}Sr$	$^{55}Mn(p,4n)^{52}Fe$	$^{58}Ni(p,\alpha)^{55}Co$
$^{nat}Ga(p,x)^{68}Ge$	$^{nat}Rb(p,x)^{82}Sr$	$^{nat}Ni(p,x)^{52}Fe$	$^{54}Fe(d,n)^{55}Co$
$^{71}Ga(p,4n)^{68}Ge$		$^{52}Cr(^{3}He,3n)^{52}Fe$	$^{56}Fe(p,2n)^{55}Co$
			$^{nat}Fe(p,x)^{55}Co$

^{61}Cu	^{66}Ga	^{68}Ga	^{90}Nb
$^{61}Ni(p,n)^{61}Cu$	$^{66}Zn(p,n)^{66}Ga$	$^{68}Zn(p,n)^{68}Ga$	$^{93}Nb(p,x)^{90}Nb$
$^{64}Zn(p,\alpha)^{61}Cu$	$^{63}Cu(\alpha,n)^{66}Ga$	$^{65}Cu(\alpha,n)^{68}Ga$	$^{89}Y(\alpha,x)^{90}Nb$

^{89}Zr	^{82}As	^{73}Se	^{76}Br
$^{nat}Y(\alpha,x)^{89}Zr$	$^{nat}Ge(p,xn)^{72}As$	$^{75}As(p,3n)^{73}Se$	$^{76}Se(p,n)^{76}Br$
$^{89}Y(p,n)^{89}Zr$		$^{72}Ge(\alpha,3n)^{73}Se$	$^{77}Se(p,2n)^{76}Br$
$^{89}Y(d,2n)^{89}Zr$			$^{75}As(\alpha,3n)^{76}Br$

CRP-III-Positron emitters- II

^{86}Y

^{86}Sr(p,n)^{86}Y

^{86}Sr(p,n)^{86}Y

^{85}Rb(α,3n)^{86}Y

^{94m}Tc

^{94}Mo(p,n)^{94m}Tc

^{92}Mo(α,x)^{94m}Tc

^{110m}In

^{110}Cd(p,n)^{110m}In

^{120}I

^{120}Te(p,n)^{12}0I

^{122}Te(p,3n)^{120}I

^{62}Zn/^{62}Cu generator

^{63}Cu(p,2n)^{62}Zn

^{72}Se/^{72}As generator

^{75}As(p,4n)^{72}Se

^{nat}Br(p,x)^{72}Se

^{140}Nd/^{140}Pr generator

^{140}Nd/^{140}Pr generator

^{118}Te/^{118}Sb generator.

^{122}Xe/^{122}I generator

^{128}Ba/^{128}Cs generator

^{110}Sn/^{110}In^{m} generator

^{44}Ti/^{44}Sc generator

CRP-III Therapeutic radioisotopes

^{67}Cu	$^{90g+m}$Y	^{64}Cu	^{186,188}Re
^{68}Zn(γ,p)^{67}Cu ^{67}Zn(n,p)^{67}Cu ^{68}Zn(n,x)^{67}Cu	^{90}Zr(n,p)$^{90g+m}$Y	^{64}Zn(n,p)^{64}Cu	^{nat}W(α,x)^{186,188}Re

CRP-III Summary

- 26 monitor reactions
- 18 reactions for γ-emitters
- 39 reactions for positron emitters (+ generators)
- 39 reactions to remeasure

Missing points and problems

- **Logical sequence**
  - **Decay data**
  - **Monitor reactions**
  - **Production reaction**
- **Missing the validation of recommended data**
- **Standard monitors need for absolute measurement and intercomparison**
- **Problem of inclusion of new, low quality data measured at low technical and expertise.**
- **Too large number of reactions**

Conclusions on data evaluation

- **Experimental data play a key role in evaluation of nuclear reaction data.**
- **The prediction capabilities of the nuclear reaction model codes is limited.**
- **Evaluation of light charged particle induced data is not well established.**
- **The requirements on the quality and on the uncertainties are lower compared to other nuclear applications.**
- **To keep the data base in good shape, continuous evaluation.**
- **The evaluation and the upgrading requires detailed information on the used nuclear data, the experimental parameters and the uncertainty of the parameters contributing to the measured value and the way of the contribution!!!**
- **The list of the radioisotopes used in nuclear medicine and biological research is continuously changing.**