Nuclear Data for Charged-particle Monitor Reactions and Medical Isotope Production

1st RCM Meeting – December 3-7, 2012

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Vienna, Austria

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- Monitor reactions – similar to neutron standards
  - ✓ measurements – exclusively using activation technique
  - ✓ cross-section evaluations & covariance's

- Nuclear Structure & Decay:
  - ✓ To support data needed for monitor reactions
  - ✓ To address also some other important issues as a consequence of previous meetings
  - ✓ Importance of improved data for Auger emitters

- consultants' meeting on "High-precision beta-intensity measurements and evaluations for specific PET radioisotopes", 3-5 September 2008, IAEA Headquarters, Vienna, Austria, IAEA report INDC(NDS)-0535, December 2008;
- consultants' meeting on "Improvements in charged-particle monitor reactions and nuclear data for medical isotope production", 21-24 June 2011, IAEA Headquarters, Vienna, Austria, IAEA report INDC(NDS)-0591, September 2011;
- technical meeting on "Intermediate-term nuclear data needs for medical applications: cross sections and decay data", 22-26 August 2011, IAEA Headquarters, Vienna, Austria, IAEA report INDC(NDS)-0596, September 2011.

Data Repository

International Atomic Energy Agency
Nuclear Data Services
قسم البيانات النووية مقدمة من

Databases » EXFOR | ENDF | CINDA | IBANDL | Medical | PGAA | NGAtlas | RIPL | FENDL | IRDF-2002 | IRDFF

Medical Applications @ Nuclear Data Section

A unified view to medical applications, databases, documents, libraries and ongoing projects

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Cross sections for diagnostic radioisotope production and beam monitor reactions

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Therapeutic Radioisotope Production

Cross sections for production of therapeutic radioisotopes

Established Nuclides...

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Therapeutic Radioisotope Production web site

MIRD

Tables of nuclear and atomic radiations from nuclear decay and decay schemes

Get (e.g. 99Tc, or 238U)

Provided by Brookhaven U.S. National Nuclear Data Center

MIRD web site

Medical Radiotherapy

PHSP - phase-space database for external beam radiotherapy

Co-60 phsp...

Photon linac phsp...

Electron linac phsp...

PHSP web site

Heavy Charged-Particle Interactions

Compiled and evaluated heavy charged-particle nuclear data for therapeutic applications

Summary Report CM 2006...

Summary Report RCM 2007...

Heavy charged-particle interaction web site

a myth & surprise …

if the data in TOI, NUDAT, ENDF-B, JEFF all agree - the data are all GOOD!

	http://nucleardata.nuclear.lu.se/nucleardata/toi/					http://www.nndc.bnl.gov/nudat2/				
Nuclide	T1/2	err		Eg keV	Ig %	T1/2	err	decay mod	Eg keV	Ig %
Sc-47	3.3492 d	0.0006	b- 100%	159.377	68.3	3.3492 d	0.0006	b- 100%	159.381	68.3
Cr-51	27.7025 d	0.0024	EC 100%	320.0824	10	27.7025 d	0.0024	EC 100%	320.0824	9.91
Mn-51	46.2 m	0.1	EC+B+ 100%			46.2 m	0.1	EC 100%	511	194.17
Mn-52	5.591 d	0.003	EC+B+ 10	1434.068	100	5.591 d	0.003	EC 100%	1434.092	100
Fe-55	2.73 y	0.03	EC 100%	125.95	1.28-e7	2.737 y	0.011	EC 100%	126	1.28E-07
Fe-59	44.503 d	0.006	b-100%	1099.251	56.5	44.495 d	0.009	b- 100%	1099.245	56.5
Co-55	17.53 h	0.03	EC+B+ 10	931.3	75	17.53 h	0.03	EC 100%	931.1	75
Co-57	271.79 d	0.09	EC 100%	122.0614	85.6	271.74 d	0.06	EC 100%	122.0607	85.6
Co-60	5.2714 y	0.0005	b-100%	1332.501	99.9856	1925.28 d	0.14	b- 100%	1332.492	99.9826
Cu-61	3.333 h	0.005	EC+B+ 10	282.956	12.2	3.333 h	0.005	EC 100%	282.956	12.2
Cu-62	9.74 m	0.02	EC+B+ 10	1172.9	0.34	9.673 m	0.008	EC 100%	1173.02	0.342
Cu-64	12.7 h	0.002	EC+B+ 61	1345.84	0.473	12.701 h	0.002	EC 61.5%	1345.77	0.475
			b-39%					b- 38.5%		
Cu-67	61.83 h	0.12	b-100%	184.577	48.7	61.83 h	0.12	b-100%	184.577	48.7
Zn-62	9.186 h	0.013	EC+B+ 10	596.56	26	9.186 h	0.013	EC 100%	596.56	26
Zn-65	244.26 d	0.26	EC+B+ 10	1115.546	50.6	243.66 d	0.09	EC 100%	1115.539	50.04
Ga-64	2.627 m	0.012	EC+B+ 10	991.56	46	2.627 m	0.012	EC 100%	991.51	46
Ga-67	3.2612 d	0.0006	EC 100%	93.311	39.2	3.2617 d	0.0005	EC 100%	93.31	38.81
Ga-68	67.629 m	0.024	EC+B+ 10	1077.35	3.0	67.71 m	0.09	EC 100%	1077.34	3.22
Ge-68	270.8 d	0.3	EC 100%			270.95 d	0.16	EC 100%		
As-72	26 h	0.1	EC+B+ 10	834.01	80	26 h	0.1	EC 100%	833.99	81
As-74	17.77 d	0.02	b- 34%	634.78	15.4	17.77 d	0.02	EC 66%	595.83	59
			EC+B+ 66	595.847	59			b- 34%	634.78	15.4

but all those came from a single source – ENSDF - so they should be the same!

TOI is 14 years old and for some mass chains ENSDF is 7-10 years old – new data is not timely included – especially those related to medical isotopes (charged particle induced reactions)

- ✓ deficiencies in the experimental decay data
- ✓ deficiencies in the evaluated data

What was discussed at the meeting

Table 1: Monitor reactions

Cross sections	Decay data	Agreed responsibilities, and actions
$^{27}Al(p,x)^{22,24}Na$	–	**ACTION**: LANL (re-assess up to 800 MeV)
$^{27}Al(d,x)^{22,24}Na$		**ACTION**: Debrecen / VUB (re-assess)
$^{27}Al(^{3}He,x)^{22,24}Na$		**ACTION**: Debrecen / VUB (re-assess)
$^{27}Al(\alpha,x)^{22,24}Na$		**ACTION**: Kim (measure); **ACTION**: Debrecen / VUB (assess)
$^{nat}Ti(d,x)^{46}Sc$	–	**ACTION**: Debrecen / VUB (re-assess)
$^{nat}Ti(^{3}He,x)^{48}V$	–	**ACTION**: Lebeda (measure and re-assess up to 46 MeV)
$^{nat}Ni(d,x)^{56,58}Co$	–	**ACTION**: Debrecen / VUB (measure and re-assess)
$^{nat}Cu(p,x)^{58}Co$	–	**ACTION**: Kim (measure); **ACTION**: LANL (measure and assess up to 100 MeV)
$^{nat}Cu(p,x)^{62,63,65}Zn$		**ACTION**: Kim (measure); Debrecen / VUB (measure and re-assess)
$^{nat}Cu(d,x)^{62,63,65}Zn$		**ACTION**: Debrecen / VUB (measure and re-assess)
$^{nat}Cu(\alpha,x)^{66,67}Ga$, ^{65}Zn		**ACTION**: Kim (measure and re-assess)
$^{nat}Mo(p,x)^{96}Tc^{g+m}$	–	**ACTION**: Debrecen / VUB / Lebeda (assess)
–	^{61}Cu	evaluate ^{61}Cu decay scheme (**ACTION**: Bé)
–	^{62}Zn	evaluate ^{62}Zn decay scheme, priority 2 (see ENSDF, 2012)
–	^{63}Zn	evaluate ^{63}Zn decay scheme (**ACTION**: Nichols)
previously evaluated cross sections	–	**ACTION**: all monitor reaction cross sections included in IAEA-TECDOC-1211 but not listed above will be re-evaluated by Debrecen / VUB to include uncertainties and covariances.

Table 2: Diagnostic γ emitters

Cross sections	Decay data	Agreed responsibilities, and actions
$^{90}Zr(n,p)^{90}Y^{g+m}$	–	**ACTION**: ITA / Nagai (measure) **- ACTION**: ITA (assess) **-** see also IRDFF (http://www-nds.iaea.org/IRDFF) and IAEA Technical Reports Series No. 473.
$^{100}Mo(n,2n)^{99}Mo$	–	**ACTION**: ITA / Nagai (assess)
$^{100}Mo(p,2n)^{99}Tc^{g+m}$		**ACTION**: Lebeda (measure); **ACTION**: ITA (assess)
$^{100}Mo(p,pn)^{99}Mo$		**ACTION**: Lebeda (measure); **ACTION**: ITA (assess)
$^{100}Mo(d,3n)^{99}Tc^{g+m}$		**ACTION**: Lebeda / ITA (assess)
$^{100}Mo(d,p2n)^{99}Mo$		**ACTION**: Lebeda / ITA (assess)
$^{100}Mo(\gamma,n)^{99}Mo$		**ACTION**: Naik / Kim (measure and assess)
$^{238}U(\gamma,f)^{99}Mo$		**ACTION**: Naik (measure and assess)
$^{68}Zn(\gamma,p)^{67}Cu$	–	**ACTION**: Naik / Kim (measure and assess)
$^{67}Zn(n,p)^{67}Cu$		**ACTION**: Nagai (measure); **ACTION**: ITA (assess) **-** see also IRDFF (http://www-nds.iaea.org/IRDFF) and IAEA Technical Reports Series No. 473.
$^{68}Zn(n,x)^{67}Cu$		**ACTION**: Nagai (measure); **ACTION**: ITA (assess)
$^{64}Zn(n,p)^{64}Cu$		**ACTION**: Nagai (measure); **ACTION**: ITA (assess) **-** see also IRDFF (http://www-nds.iaea.org/IRDFF) and IAEA Technical Reports Series No. 473, and INDC(NDS)-0526, August 2008
$^{112}Cd(p,2n)^{111}In$	–	**ACTION**: Debrecen / VUB (assess)
$^{124}Xe(p,x)^{121}I$	–	**ACTION**: Debrecen / VUB (assess)
$^{124}Xe(p,2n)^{123}Cs$	–	**ACTION**: Debrecen / VUB (assess)
$^{124}Xe(p,pn)^{123}Xe$		**ACTION**: Debrecen / VUB (assess)
$^{51}V(p,n)^{51}Cr$	–	**ACTION**: Debrecen (re-assess all noted production routes of ^{51}Cr)

Table 2: Diagnostic γ emitters (cont'd)

Cross sections	Decay data	Agreed responsibilities, and actions
$^{203}Tl(p,2n)^{202}Pb^{m}$	–	**ACTION**: Debrecen / VUB (re-assess)
$^{203}Tl(p,3n)^{201}Pb$		**ACTION**: Debrecen / VUB (re-assess)
$^{203}Tl(p,4n)^{200}Pb$		**ACTION**: Debrecen / VUB (re-assess)
$^{nat}W(\alpha,x)^{186,188}Re$	–	**ACTION**: Kim (measure and assess)
–	^{67}Cu	**ACTION**: Kondev (measure, and evaluate decay scheme)
–	$^{99}Tc^{m}$	**ACTION**: Kibedi and Kondev (Auger-electron data)
–	^{111}In	**ACTION**: Kibedi and Kondev (Auger-electron data)

Table 3: Positron emitters

Cross sections	Decay data	Agreed responsibilities, and actions
$^{55}Mn(p,4n)^{52}Fe$	–	**ACTION**: Lahore (assess)
$^{nat}Ni(p,x)^{52}Fe$		**ACTION**: Lahore (assess)
$^{52}Cr(^{3}He,3n)^{52}Fe$		**ACTION**: Lahore (assess)
$^{58}Ni(p,\alpha)^{55}Co$	–	**ACTION**: Lahore (assess)
$^{54}Fe(d,n)^{55}Co$		**ACTION**: Lahore (assess)
$^{56}Fe(p,2n)^{55}Co$		**ACTION**: Lahore (assess)
$^{nat}Fe(p,x)^{55}Co$		**ACTION**: Kim (measure); **ACTION**: Lahore (assess)
$^{61}Ni(p,n)^{61}Cu$	–	**ACTION**: Jülich (measure and assess)
$^{64}Zn(p,\alpha)^{61}Cu$		**ACTION**: Lebeda (measure and assess)
$^{66}Zn(p,n)^{66}Ga$	–	**ACTION**: Lahore (assess)
$^{63}Cu(\alpha,n)^{66}Ga$		**ACTION**: Lahore (assess)
$^{68}Zn(p,n)^{68}Ga$	–	**ACTION**: Jülich (measure and assess)
$^{65}Cu(\alpha,n)^{68}Ga$		**ACTION**: Jülich (assess)
$^{93}Nb(p,x)^{90}Nb$	–	**ACTION**: Kim (measure and assess)
$^{89}Y(\alpha,x)^{90}Nb$		**ACTION**: Kim (measure and assess)
$^{89}Y(\alpha,x)^{89}Zr$		**ACTION**: Kim (measure and assess)
$^{nat}Ge(p,xn)^{72}As$	–	**ACTION**: Jülich (measure); **ACTION**: Lahore (assess)

Table 3: Positron emitters (cont'd)

Cross sections	Decay data	Agreed responsibilities, and actions
$^{75}As(p,3n)^{73}Se$	–	**ACTION**: Lebeda (measure); **ACTION**: Lahore (assess)
$^{72}Ge(\alpha,3n)^{73}Se$		**ACTION**: Lahore (assess)
$^{76}Se(p,n)^{76}Br$	–	**ACTION**: Jülich (measure); **ACTION**: Lahore (assess)
$^{77}Se(p,2n)^{76}Br$		**ACTION**: Jülich (measure); **ACTION**: Lahore (assess)
$^{75}As(\alpha,3n)^{76}Br$		**ACTION**: Lahore (assess)
$^{86}Sr(p,n)^{86}Y$	–	**ACTION**: Lahore (assess)
$^{88}Sr(p,3n)^{86}Y$		**ACTION**: Lahore (assess)
$^{85}Rb(\alpha,3n)^{86}Y$		**ACTION**: Lahore (assess)
$^{89}Y(p,n)^{89}Zr$	–	**ACTION**: ITA (assess)
$^{89}Y(d,2n)^{89}Zr$		**ACTION**: Lebeda (measure and assess)
$^{94}Mo(p,n)^{94}Tc^{m}$	–	**ACTION**: ITA (assess)
$^{92}Mo(\alpha,x)^{94}Tc^{m}$		**ACTION**: ITA (assess)
$^{110}Cd(p,n)^{110}In^{m}$	–	**ACTION**: Debrecen / VUB (assess)
$^{120}Te(p,n)^{120}I$	–	**ACTION**: Lahore (assess)
$^{122}Te(p,3n)^{120}I$		**ACTION**: Lahore (assess)
–	^{52}Fe	evaluate, and assess if new measurements required, priority 3 (**ACTION**: Luca – evaluate decay scheme)
–	^{64}Cu	discrepancy in the intensity of weak gamma line (**ACTION**: Bé – re-evaluate decay scheme)
–	^{66}Ga	determine positron intensities and evaluate, priority 1 (**ACTION**: Kondev – measure, and evaluate decay scheme)
–	^{72}As	determine positron intensities and evaluate, priority 2 (no volunteer)

Table 3: Positron emitters (cont'd)

Cross sections	Decay data	Agreed responsibilities, and actions
–	^{73}Se	determine positron intensities and evaluate, priority 2 (**ACTION**: Nichols – evaluate decay scheme)
–	^{76}Br	determine positron intensities and evaluate, priority 3 (**ACTION**: Nichols – evaluate decay scheme)
–	^{86}Y	PET analogue of therapeutic ^{90}Y; determine positron intensities and evaluate, priority 1 (**ACTION**: Kondev - measure, and evaluate decay scheme)
–	^{89}Zr	evaluate ^{89}Zr decay scheme, priority 3 (**ACTION**: Nichols)
–	$^{94}Tc^{m}$	PET analogue of therapeutic $^{99}Tc^{m}$; evaluate $^{94}Tc^{m}$ decay scheme, priority 2 (**ACTION**: Nichols)
–	^{120}I	evaluate ^{120}I decay scheme, priority 3 (**ACTION**: Nichols)

Table 3: Positron emitters (cont'd.): generators

Generator	Cross sections	Decay data	Agreed responsibilities, and actions
$^{62}Zn/^{62}Cu$		–	PET analogue of therapeutic ^{67}Cu
	$^{63}Cu(p,2n)^{62}Zn$		**ACTION**: Debrecen / VUB (measure and assess)
$^{68}Ge/^{68}Ga$		–	PET analogue of proposed/new therapeutic ^{67}Ga
	$^{nat}Ga(p,xn)^{68}Ge$		**ACTION**: Debrecen / VUB (measure and assess)
	$^{69}Ga(p,2n)^{68}Ge$		**ACTION**: Debrecen / VUB (measure and assess)
	$^{71}Ga(p,4n)^{68}Ge$		**ACTION**: Debrecen / VUB (measure and assess)
$^{72}Se/^{72}As$	$^{75}As(p,4n)^{72}Se$	–	**ACTION**: LANL (assess)
	$^{nat}Br(p,x)^{72}Se$		**ACTION**: LANL (assess)
$^{82}Sr/^{82}Rb$	$^{nat}Rb(p,xn)^{82}Sr$ $^{85}Rb(p,4n)^{82}Sr$	–	**ACTION**: LANL (assess)
$^{52}Fe/^{52}Mn^{m}$	$^{55}Mn(p,4n)^{52}Fe$ $^{nat}Ni(p,x)^{52}Fe$ $^{52}Cr(^{3}He,3n)^{52}Fe$	–	**ACTION**: Lahore (assess)
$^{110}Sn/^{110}In^{m}$	Main reactions leading to the parent nucleus	–	PET analogue of therapeutic ^{111}In and $^{114}In^{m}$; **ACTION**: Debrecen / VUB (assess)
$^{128}Ba/^{128}Cs$	Main reactions leading to the parent nucleus	–	PET analogue of proposed/new therapeutic ^{131}Cs; **ACTION**: Debrecen / VUB (assess)
$^{122}Xe/^{122}I$	Main reactions leading to the parent nucleus	–	PET analogue of therapeutic ^{123}I, ^{125}I and ^{131}I; **ACTION**: Debrecen / VUB (assess)
$^{118}Te/^{118}Sb$	Main reactions leading to the parent nucleus	–	PET analogue of proposed/new therapeutic ^{117}Sb and ^{119}Sb; **ACTION**: Debrecen / VUB (assess)
$^{140}Nd/^{140}Pr$	Main reactions leading to the parent nucleus	–	**ACTION**: LANL (assess)
$^{44}Ti/^{44}Sc$	Main reactions leading to the parent nucleus	half-life of ^{44}Ti	**ACTION**: Jülich (assess cross sections); **ACTION**: Kondev (evaluate ^{44}Ti half-life)

Table 4: Therapeutic α emitters

Cross sections	Decay data	Agreed responsibilities, and actions
$^{229}Th(\alpha)^{225}Ra(\beta^-)^{225}Ac(\alpha)$ decay chain to ^{213}Bi:	–	Decay chain recently reevaluated in Actinide decay data CRP (to be published).
$^{232}Th(p,x)^{225}Ra$		**ACTION**: LANL (assess)
$^{232}Th(p,x)^{225}Ac$		**ACTION**: LANL (assess)
$^{226}Ra(p,2n)^{225}Ac$		**ACTION**: LANL (assess)
$^{232}Th(p,x)^{227}Ac$		**ACTION**: LANL (assess)
$^{230}U(\alpha)^{226}Th(\alpha)$ decay chain:	–	
$^{231}Pa(d,3n)^{230}U$		**ACTION**: Lebeda (assess)
$^{231}Pa(p,2n)^{230}U$		**ACTION**: Lebeda (assess)
$^{232}Th(p,3n)^{230}Pa(\beta^-)^{230}U$		**ACTION**: Lebeda (assess)
$^{227}Th(\alpha)^{223}Ra(\alpha)$ decay chain	–	
$^{232}Th(p,x)^{227}Th$		**ACTION**: LANL (assess)
–	^{230}U decay chain	**ACTION**: Luca and Bé (evaluate decay schemes of radionuclides in ^{230}U decay chain: $^{230}U(\alpha)^{226}Th(\alpha)^{222}Ra(\alpha)^{218}Rn(\alpha)^{214}Po(\alpha)^{210}Pb(\beta^-)^{210}Bi(\beta^-)^{210}Po(\alpha)^{206}Pb$(stable))

Table 5: Electron and X-ray emitters

Cross sections	Decay data	Agreed responsibilities, and actions
$^{130}Ba(n,\gamma)^{131}Ba(EC)^{131}Cs$	–	**ACTION**: Nagai (assess)
$^{131}Xe(p,n)^{131}Cs$	–	**ACTION**: Debrecen / VUB (measure and assess)
$^{133}Cs(p,3n)^{131}Ba(EC)^{131}Cs$	–	**ACTION**: Debrecen / VUB (measure and assess)
$^{176}Hf(\alpha,2n)^{178}W(EC)^{178}Ta$	–	**ACTION**: Kim (measure and assess)
$^{nat}Hf(p,x)^{178}Ta$	–	**ACTION**: Kim (measure and assess)
–	^{178}Ta	**ACTION**: Kibedi and Kondev (Auger-electron data)
–	^{103}Pd	evaluate ^{103}Pd decay scheme, priority 1 (**ACTION**: Chechev (evaluate decay scheme) and Nichols (review evaluation); **ACTION**: Kibedi and Kondev (Auger-electron data))
–	–	Capote, **ACTION**: establish link to neutron-induced production data, and implement additional changes to IAEA Medical Portal

Consultants' Meeting on Auger Electron Emission Data Needs for Medical Applications

IAEA Headquarters, Vienna, Austria 9 – 10 May 2013

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Consultants' Meeting

"Auger electron emission data needs for medical applications"

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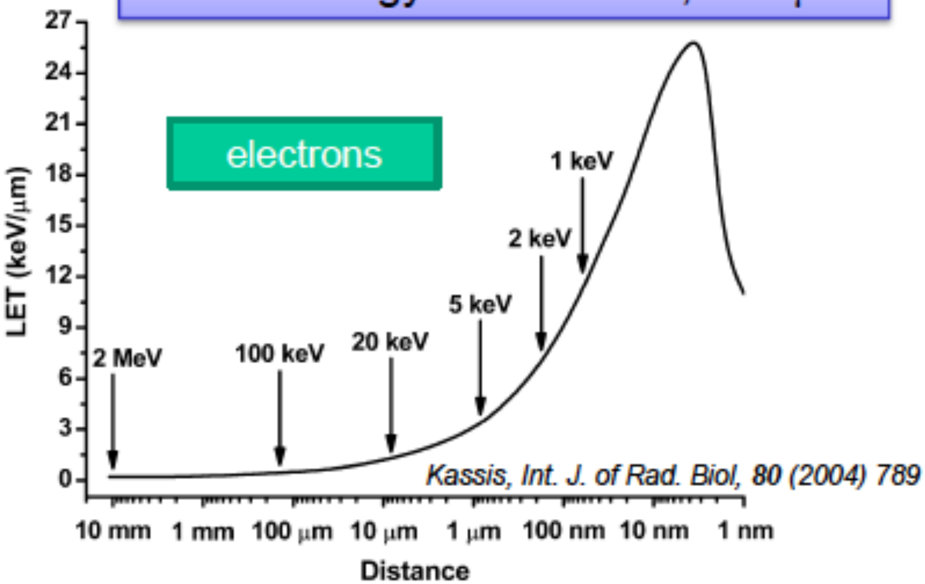
Regaud and Lacassagne (1927)

"The ideal agent for cancer therapy would consist of heavy elements capable of emitting radiations of molecular dimensions, which could be administered to the organism and selectively fixed in the protoplasm of cells one seeks to destroy."

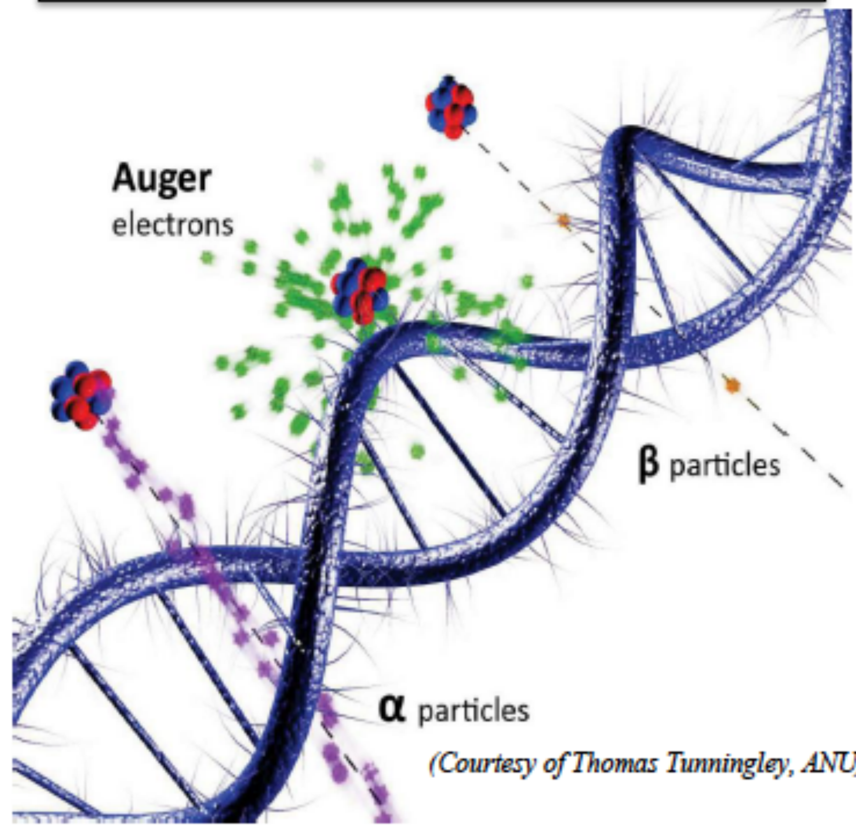
Targeted tumor therapy

Biological effect:

Linear energy transfer **LET**, keV/µm



Kassis, Int. J. of Rad. Biol, 80 (2004) 789



(Courtesy of Thomas Tunningley, ANU).

	RADAR	DDEP	Eckerman & Endo (2007)	Howell (1992)	Stepanek (2000)	Pomplun (2012)
Nuclear decay data	ENSDF	DDEP	ENSDF	ENSDF	ENSDF	ICRP38
Conversion coefficients	Hslcc	Rplcc/Brlcc	Rplcc, 1978 Band	Rplcc	2000 Stepanek	Hslcc, 1971 Dragoun, 1976 Band
Electron Capture Ratios	1971 Gove & Martin	1995 Schönfeld	1977 Bambynek	1971 Gove & Martin, 1970Martin	1971 Gove & Martin, 1970Martin	1971 Gove & Martin
Atomic transition rates	1972 Bambynek, RADLST	1974 Scofield, 1995 Schönfeld & Janßen, 2006 Be et al., EMISSION	1991 Perkins, EDISTR04	1979 Chen, 1972/1975 McGuire, 1983 Kassis, 1974 Scofield, 1974 Manson & Kenedy	1991 Perkins	1979 Chen, 1972/1975 McGuire, 1970 Storm & Israel, 1979 Krause
Atomic transition energies	1970 Bearden & Burr, Neutral atom	1977 Larkins, Semi-empirical	1991 Perkins, Neutral atom	Z/Z+1 (Auger), Neutral atom (X-ray)	Dirack-Fock calculation	1991 Desclaux, Dirack-Fock calculation
Vacancy propagation	**Deterministic**	**Deterministic**	**Deterministic (+++)**	**Monte Carlo with charge neutralization**	**Monte Carlo**	**Monte Carlo**

	RADAR	DDEP	Eckerman & Endo (2007)	Howell (1992)	Stepanek (2000)	Pomplun (2012)
^{99m}Tc (6.007 h)	0.869	0.13	4.363	4.0		2.5
^{111}In (2.805 d)	1.136	1.16	7.215	14.7	6.05	
^{123}I (13.22 h)	1.064	1.08	13.71	14.9		6.4
^{125}I (59.4 d)	1.77	1.78	23.0	24.9	15.3	12.2
^{201}Tl (3.04 d)	0.773	0.614	20.9	36.9		
Vacancy propagation	Deterministic	Deterministic	Deterministic (+++)	Monte Carlo with charge neutralization	Monte Carlo	Monte Carlo

Common problems / limitations

- In some cases neutral atom binding energies are used for atoms with vacancies; i.e. for ions
- Single initial vacancy is considered. Secondary vacancies are ignored
- Atomic radiations only from primary vacancies on the K and L shell
- Limited information on sub-shell rates
- Auger electrons below ~1 keV are often omitted

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Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1 – 100

S. T. Perkins, D. E. Cullen, M. H. Chen,
J. H. Hubbell (National Institute of Standards and Technology), J. Rathkopf, J. Scofield

Assumptions and Approximations

This library contains data for subshells that are occupied when an atom is in its neutral, ground state. Data are not included for initially ionized or excited atoms.

The library does not describe the electron that is emitted when the atom is initially ionized. It is assumed that this electron has been explicitly accounted for based on the kinematics of the ionizing event, e.g., photoelectric, electron impact ionization, or internal conversion. It is also assumed that once ionized, the relaxation is independent of how the atom was initially ionized.

The relaxation data in the library is designed to describe the bound-bound radiative and nonradiative transitions following an ionization event. Additionally it is assumed that relaxation only occurs where both radiative and nonradiative transitions are possible.

It is also assumed that the binding energy of all subshells are the same for neutral ground state atoms as for ionized atoms. This assumption has been adopted because at the current time there is no provision to provide complete data describing the binding energy of each subshell of an atom when any of its other subshells is singly or multiply ionized.

X-rays

6. J. H. Scofield, private communication, Lawrence Livermore National Laboratory, Livermore, CA (1988).
7. J. H. Scofield, *Phys. Rev.* **179**, 9 (1969).
8. J. H. Scofield, *At. Data Nuc. Data Tables*, **14**, 121 (1974) 8
9. J. H. Scofield, "Radiative Transitions," in *Atomic Inner Shell Processes*, Chapt. VI, Bernard Craseman, ed. (Academic Press, 1973).

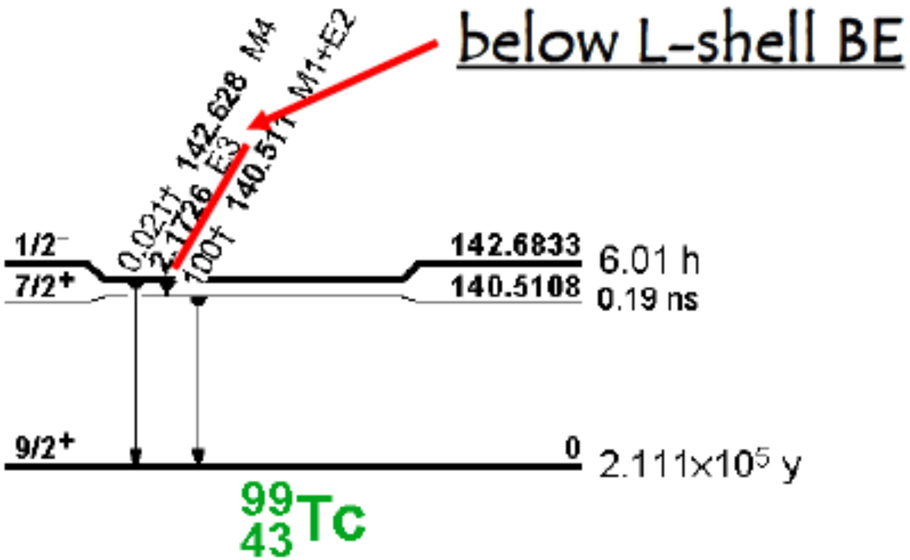
Auger electrons

10. M. H. Chen, private communication, Lawrence Livermore National Laboratory, Livermore, CA (1988).
11. H. H. Chen et al., *Phys. Rev. A* **19**, 2253 (1979).
12. M. H. Chen, B. Craseman, and H. Mark, *Phys. Rev. A* **21**, 449 (1980).
13. M. H. Chen, B. Craseman, and H. Mark, *At. Data Nucl. Data Tables* **24**, 13 (1979) .
14. M. H. Chen, B. Craseman, and H. Mark, *Phys. Rev. A* **24**, 177 (1981).
15. M.H. Chen, B. Craseman, and H. Mark, *Phys. Rev. A* **24**, 13 (1979).
16. M. H. Chen, B. Craseman, and H. Mark, *Phys. Rev. A* **27**, 2989 (1983).

- **Initial state:** neutral isolated atom
- **Nuclear structure data:** from ENSDF
- **Electron capture (EC) rates:** Schönfeld (1998Sc28)
- **Internal conversion coefficients (ICC):** BrIcc (2008Ki07)
- **Auger and X-ray transition rates:** EADL (1991 Perkins)

  Calculated for single vacancies!
- **Auger and X-ray transition energies:** RAINE (2002Ba85)

  Calculated for actual electronic configuration!
- **Vacancy creation and relaxation from EC and IC:** treated independently
- ***Ab initio* treatment of the vacancy propagation:**
  - Transition energies and rates evaluated on the spot
  - Propagation terminated once the vacancy reached the valence shell



1 photon per 1.37×10^{10} decays!

BrIccS v2.3 (9-Dec-2011)

Z=43 (Tc, Technetium)

γ-energy: 2.1726 keV

Data Sets: BrIccFO

Shell	E(ce)	E3
Tot		1.370E10 (20)
M1	1.63	2.26E6 (4)
M2	1.73	3.37E9 (5)
M3	1.75	5.98E9 (9)
M4	1.92	1.100E9 (16)
M5	1.92	1.655E9 (24)
M-tot	1.78	1.211E10 (17)
N1	2.10	5.00E5 (7)
N2	2.13	4.92E8 (7)
N3	2.14	8.77E8 (13)
N4	2.17	9.11E7 (13)
N5	2.17	1.350E8 (19)
N-tot	2.14	1.596E9 (23)
O1	2.17	3.49E4 (5)
O-tot	2.17	3.49E4 (5)

	DDEP	BrIccEmis
$K\alpha_1$	18.3672 ***4.21E-2***	18.421 ***4.05E-2***
$K\alpha_2$	18.251 ***2.22E-2***	18.302 ***2.13E-2***
$K\beta$	20.677 ***1.30E-2***	20.729 ***1.18E-2***
L	[2.134:3.002] ***4.82E-3***	2.466 ***4.72E-3***
M		0.263 ***7.83E-4***
N		0.047 ***8.73E-1***

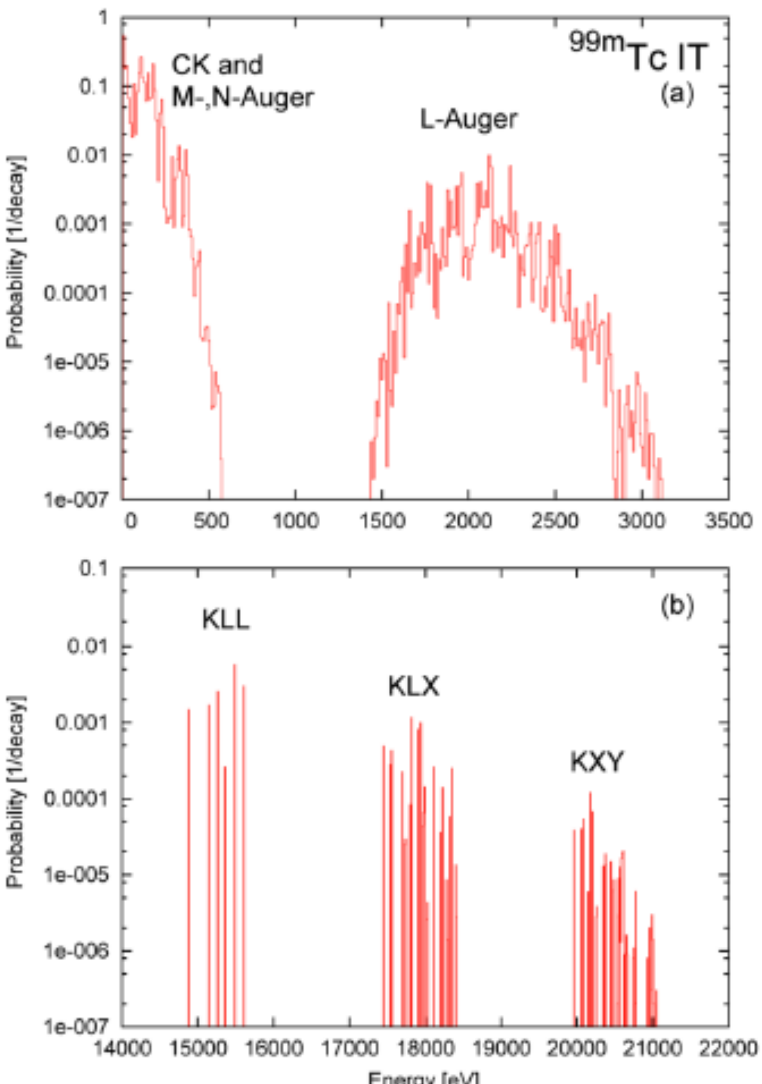
	DDEP	BrIccEmis
CK MMX		0.104 ***7.10E-1***
MXY		0.170 ***1.10E+0***
Super CK NNN		0.014 ***5.36E-1***
CK NNX		0.012 ***8.45E-1***
Total yield Auger electron per nuclear decay	***0.13***	***3.37***
RADAR (2013)	***0.869***	
Eckerman and Endo (2007)	***4.363***	
Howell (1991)	***4.0***	
Pomplun (2012)	***2.5***	

~95%
below 500 eV

Technetium-99m is used in 20 million diagnostic nuclear medical procedures every year (Wikipedia)

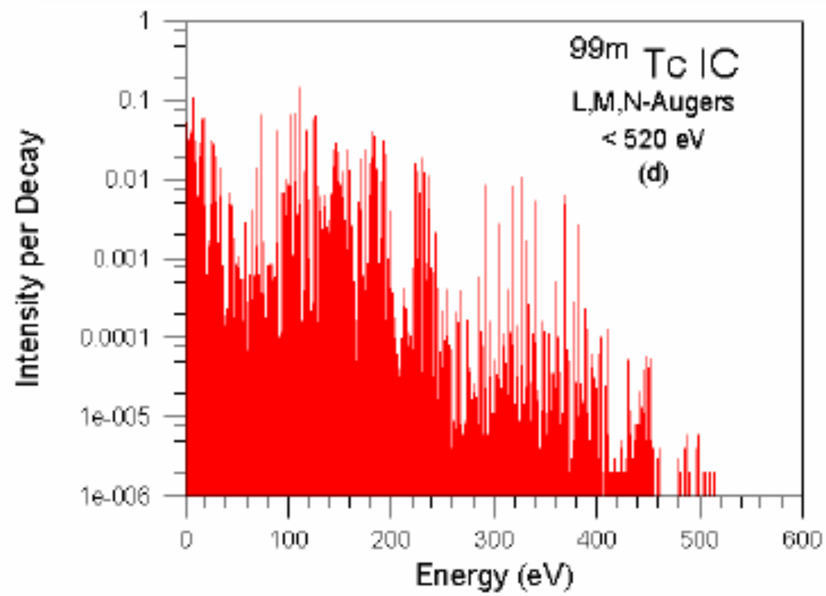
BrIccEmis:

- 10 M simulated decay events
- 455 type of Auger transitions (EADL: 273)



2012Le09 Lee et al., Comp. Math. Meth. in Medicine, v2012, Art. ID 651475

Low energy Auger electrons



B.Q. Lee, Honours Thesis, ANU 2012

- X-ray and Auger electron energy spectra evaluated using Monte Carlo approach for vacancy propagation; reasonable agreement with other models and experiments
- Problems:
  Auger energies over-estimated
  EADL atomic rates are calculated for <u>single vacancies</u>

<u>Plans and recommendation</u>

- Calculation of Atomic transition energies and rates for each propagation step using GRASP2k/RATIP
- Experimental data urgently needed to verify transition rates and energies
- Auger data for a large range of radioisotopes (beyond the medical ones)
- Auger data from "non-nuclear' excitations