



2358-12

Joint ICTP-IAEA Workshop on Nuclear Structure Decay Data: Theory and Evaluation

6 - 17 August 2012

ENSDF Analysis and Utility Codes

T.D. Johnson Brookhaven National Laboratory USA

ENSDF Analysis and Utility Codes

T.D. Johnson National Nuclear Data Center Brookhaven National Laboratory, USA





ENSDF Analysis and Utility Codes

Platforms

- Overview of the Programs
- Programs Used for Various Types of ENSDF Datasets
 - All Types of Datasets
 - Adopted
 - Decay
 - Reaction
- Additional Notes on Some of the Codes





ENSDF Analysis and Utility Codes Platforms

- Most of the programs are available for the following:
 - ANSI standard Fortran 77 or Fortran 95
 - LINUX and UNIX (gnu f77 FORTRAN, INTEL FORTRAN 90, or Lahey/Fujitsu FORTRAN 95)
 - Windows 95/98/ME/NT/2000/XP/VISTA (COMPAQ/DEC Visual Fortran)
- For LINUX, UNIX, and Windows, executables are also provided.





ENSDF Analysis and Utility Codes Overview

- ADDGAM Adds gammas to an adopted dataset
- ALPHAD Calculates αR_0 's, Hindrance Factors and theoretical $T_{\gamma_2}(\alpha)$'s
- Brlcc/HSICC (Band-Raman Internal Coefficients/ Hager-Seltzer Internal Conversion) — Interpolates internal conversion coefficients – Brlcc adopted.
- BrlccMixing Calculates mixing ratios from internal conversion coefficients
- COMTRANS (Comments Translation) Translates comment records in ENSDF dataset to a "rich text" format
- DELTA Analyzes angular correlation data
- ENSDAT (Evaluated Nuclear Structure Drawings and Tables) — Produces high quality drawings and tables in the Nuclear Data Shoots style

Data Sheets style Brookhaven Science Associates U.S. Department of Energy





ENSDF Analysis and Utility Codes Overview - 3

- RadList (Radiation Listing) Calculates atomic & nuclear radiations. Checks energy balance
- RULER Calculates reduced transition probabilities
- TREND (Tabular Representation of ENSDF) Tabular display of ENSDF data





ENSDF Analysis and Utility Codes All Types of Datasets

- Applicable programs are FMTCHK, ENSDAT, PANDORA, and TREND.
- FMTCHK should be run after any manual changes to the file.
- ENSDAT may be used to visually check the data.
- If you are considering combining several datasets (e.g., from XUNDL), PANDORA may be useful.
- TREND may be used to visually check the data.





ENSDF Analysis and Utility Codes Adopted Levels, Gamma Datasets — 1

- Applicable programs are ADDGAM, GTOL, Brlcc, PANDORA, and RULER.
- ADDGAM and PANDORA are useful in constructing the dataset.
- PANDORA used iteratively to aid in physics decisions, checking assignments, and updating source datasets based on changes in the adopted data.
- GTOL useful only in obtaining the least-squares adjustment of the level energies.
 - Matrix may occasionally be singular.





ENSDF Analysis and Utility Codes Adopted Levels, Gamma Datasets — 2

RULER may be used in either of two modes:

- Comparison mode to provide additional information in obtaining γ -multipolarity assignments.
- Should also be run to provide the BE λ W's and BM λ W's.
- Brlcc/HSICC should be run before RULER.
- Brlcc should be run to provide the internal conversion coefficients.
 - Note that there is no need to delete the "S G" records generated by code.





- Applicable programs are ALPHAD (for α decay), GABS, GTOL, BrIcc, LOGFT (for β[±]/ε decay), RadList, and RULER.
- ALPHAD should be used to obtain the hindrance factors and, for even-even ground-state nuclei, R₀. For other nuclei, an R₀ must be supplied.
- GABS may be used to combine the data from up to three sources to obtain I_y-normalization (NR), the branching ratios (BR), and absolute I_y's.
 - BrIcc should run on the input data or the α 's from the adopted dataset should be used.





GTOL may be used to:

- Provide a least-squares adjustment of the level energies.
- Check the uncertainties and placement of the γ 's.
- Obtain the intensities of particles feeding the levels.
 Should be done before ALPHAD and LOGFT are employed.
- May be useful in deriving I_{γ} -normalization (NR).
- Brlcc may be used to:
 - Check experimentally measured α 's against theory.
 - If the adopted α 's are not used, to produce this information for the data set.





- LOGFT is required to obtain the log ft's, I_{β^+} and I_{ϵ} , and partial electron-capture fractions.
 - Should be done before using RadList.
 - If one is not using measured intensities, GTOL should be used to obtain $I_{\beta_{\text{-}}}$ and $I_{\epsilon+\beta+}.$
- RadList should be used to:
 - Check the calculated energy deposited with that based the Q-value and branching ratio.
 - To compare to experimentally obtained X-ray intensities
 - Check results against integral measurements (e.g., $\langle E_{\beta\pm} \rangle$)
 - Unresolved discrepancies should be noted in the dataset.
 - Brlcc and LOGFT should have been used before doing these checks.





RULER may be used to check or further limit multipolarities based on other methods (e.g., from experimental conversion coefficients).





- Applicable programs are GTOL, Brlcc, and RULER.
 - For (thermal n,γ) datasets, RadList may also prove of use.
- GTOL's primary use is to do a least-squares adjustment of the level energies and to check the uncertainties and placement of the γ 's.
 - If ΔE_{γ} 's are not given and a good estimate of these cannot be obtained, it may be better to use the authors' level energy values.
 - Also useful for checking for intensity imbalance problems if relative intensities are given.





- Brlcc may be used to check experimentally measured α's against theory.
 - Very useful to include α 's and partial α 's for (thermal n, γ) datasets.
- RadList may be used to check the energy balance of (thermal n,γ) datasets by tricking it.
 - Change the DSID on the ID record to indicate IT decay
 - Add an appropriate Parent record (E_{level}=S_n)
 - Add a BR of 1.0 on the Normalization record.





ENSDF Analysis and Utility Codes Additional Notes - 1

COMTRANS

- Should <u>not</u> be run on ENSDF or XUNDL files submitted to the NNDC.
 - $\ ^A4 \rightarrow A4 \rightarrow A\{-4\} \rightarrow a\{-4\}$
 - $T \rightarrow T\{-1/2\} \rightarrow T\{-1/2\}T\{-1/2\}T\{-1/2\}T\{-1/2\}T\{-1/2\}T\{-1/2\}T\{-1/2\} \rightarrow \dots$
- Useful to run before using Isotope Explorer 2 or ENSDAT.
- ENSDAT
 - Keynumber list generated by ENSDAT may be used to check the keynumbers
 - Layout commands may be embedded in the input.
 - See ENSCOMDS.TXT
 - Need to be removed before submission to the NNDC
 - "View" option available if you have a PostScript viewer such as GhostView installed.





ENSDF Analysis and Utility Codes Additional Notes - 2

- NSDFLIB Subroutine package used in all programs, except DELTA, GABS, and LWEIGHT
 - ANSI standard FORTRAN77
 - ANSI standard FORTRAN95 with a couple of exceptions
- RadList
 - · Calculated uncertainties may be overestimated.
 - Total energy deposited by γ 's calculated as $\Sigma BR \times NR \times E_{\gamma} \times I_{\gamma}$ instead of $BR \times NR \Sigma E_{\gamma} I_{\gamma}$.
 - Uses the first partial conversion coefficient found.
 - If EKC is encountered before KC, EKC will be used in the calculations.





ENSDF Analysis Detailed Alphad

Hinderance Factor — HF

- Experimental $T_{1/2}(\alpha)$ /Theoretical $T_{1/2}(\alpha)$
- Theoretical value from 1947Pr17 (M.A. Preston)
- Assumption is that 0⁺ to 0⁺ from even-even nuclei are fastest (HF = 1)
- Radius parameter (r₀) calculations
 - Alphad calculates r₀ for decays from even-even nuclei
 - See 1998Ak04 (Y.A. Akovali) for even-even values
 - Evaluator must interpolate to obtain odd-even and odd-odd cases and add to ENSDF file for alphad to calculate HF





alphad Obtaining the radius parameter

Odd N

 $r_0(Z,N) = [r_0(Z,N-1) + r_0(Z,N+1)]/2$

Odd Z

$$r_0(Z,N) = [r_0(Z-1,N) + r_0(Z+1,N)]/2$$

Odd-Odd

 $\begin{aligned} r_0(Z,N) &= [r_0(Z-1,N+1) + r_0(Z-1,N-1) + r_0(Z+1,N+1) + r_0(Z+1,N-1)]/4 \end{aligned}$





alphad More on hinderance factors

- Odd-odd and even-odd nuclei have relatively longer half-lives than theoretical calcs (I=0 decay) due to hinderance factors
- GS transition from odd nucleus can only take place if the unpaired nucleon becomes part of the α particle, and so a pair is broken





alphad Hinderance factors

1-4

- "favored". Alpha assembled from low lying pairs of nucleons in parent nucleus
- **4**-10
 - Mixing or favorable overlap between initial and final nuclear states
- **10-100**
 - Spin projs parallel but Ψ overlap not favorable
- **100-1000**
 - Change in parity, parallel spin projs
- > 1000 (change in parity, not parallel spin projs)





alphad Example ENSDF

	cm249	.al	.pha											
	249CM		253CF A D	ECA	Y		1	968BE21			11ND)S	201108	
	249CM	Н	TYP=FUL\$A	UT=I	KHALIFEN	ABUS	ALEEM\$	CIT=NDS	112,	2129	(2011)\$			
	249CM2	Н	CUT=31-De	c-2	010\$									
	249CM	Ν	1			0.	0031 4							
J	253CF	Ρ	0.0		7/2+		1	7.81 D	8		6126		4	
	2 <mark>53CF (</mark>	сР	\$Q from 2	011	AuZZ, 20	009AuZ	Z and 2	2003Au03	3					
	249CM	С	J({+253}C	fg	.s.)=7/2	2+, th	erefor	e, the f	favor	ed a b	oranch			
	249CM2	С	(HF=1.3 {	I2}) is unl	likely	to go	to the	{+24	9}Cm g.	s with J=1.	./2 (+).	
	249CM3	С	It most p	rob	ably fee	eds th	e 48-k	eV (7/2-	+) st	ate.				
	249CM	сA	E	Re	commende	ed val	ue fro	m 1991Ry	y01,	based o	on adjusted	l val	ues	
	249CM2	сA	from 1968	Be2	1, 1966F	Rg01;	2009Au	ZZ						
	249CM	сA	IA	Re	commende	ed val	ue fro	m 1991Ry	y01,	based o	on measurem	lents	of	
	249CM2	сA	1968Be21	and	1966Rg(01								
	249CM	сA	HF	r{	-0}({+24	19}Cm)	=1.509	{I5}						
	249CM	L	0.0		1/2(+)									
	249CM	L	48.758		(7/2+)			23 US						
	249CM	cL	Т	fr	om delay	yed co	in (19	66As12)						
	249CM	Α	5980	4	94.7	9 1.	32							
	249CM	L	110	1	(9/2+)									
	249CM	Α	5920	5	5.3	19 11	5							





Beta and EC decay: logft

- Needs logft.dat for radial wave function data
 - On Windows or Linux, is contained in the compressed file
 - Also under "Input data" on the main logft website.





Example of before logft

tl205noft.beta												
205TL		205HG E	- DECAY	Y		19	971HI01			04NDS	200404	
205TL	H	TYP=FUI	\$AUT=F	.G. KOl	NDEV\$CI	T=NDS	101, 5	21	(2004) \$CUT=1	-Feb-2004\$		
205TL	сG	cG E,RI\$From 1971Hi01, unless otherwise specified.										
205TL	сG	; M,MR\$From adopted gammas, unless otherwise specified.										
205TL	cL	L E\$From a least-squares fit to E g.										
205TL	cL	J\$From	adopted	d level	ls.							
205HG	Ρ	0.0	1	1/2-		5	.14 M	9		1533	4	
205TL	N	0.022	10		1		1.0					
205TL	205TL cN NR\$based on I b{+-}=3.2% {I15} to the 203.7 level.											
205TL2	205TL2cN The total energy realized in b{+-} decay of {+205}Hg is calculated											
205TL3	TL3cN using RADLST as											
205TL4	205TL4cN 1534 keV {I23}. This value is in a very good agreement with											
205TL5	205TL5cN Q(g.s.)=1533 keV {I4}, thus suggesting that the decay scheme											
205TL6	6cN	is comp	lete.									
205TL	L	0.0	1	1/2+								
205TL	В		(96.8	15							
205TL	L	203	.6519 3	3/2+		1	.46 NS	8				





After logft (logft.new)





