



UNIVERSIDAD MICHOCANA
DE SAN NICOLÁS DE HIDALGO

Predictability analysis of α decay formulae and the α partial half-lives of exotic nuclei

Nabanita Dasgupta-Schubert

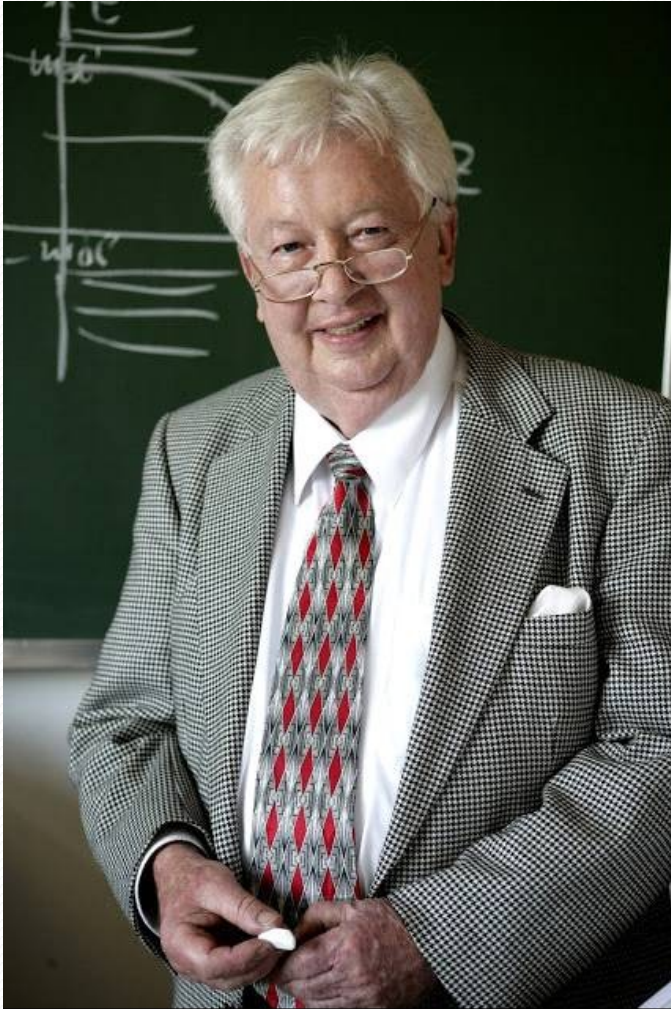
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Prof. Dr. Walter Greiner, 1935- 2016



Lawrence Livermore National
Laboratory, USA



Frankfurt Institute of Advanced Study,
Germany



Greiner's contribution to radioactivity studies

- Starting from the 1980s, Dorin Poenaru, Walther Greiner and colleagues developed and refined an analytical formula that unified alpha and cluster radioactivities under the umbrella of super asymmetric spontaneous fission (ASAF/UNIV formula). (D. N. Poenaru and W. Greiner (1999) Numerical and Analytical Super-Asymmetric Fission Model for Exotic Cluster Decays. Heavy Elements and Related New Phenomena: pp. 673-729)
- Quantum mechanical barrier tunneling and the WKB approximation used to evaluate the alpha half-life, T_α
- Alpha preformation probability, a deformation/Coulomb potential energy barrier as well as empirical hindrance factors for nuclides with odd nucleon numbers
- Main shell effect accounted for through Q . However discrepancies in the predicted T_α at or near shell closures, particularly at $N=126$.



Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																													
1 H Hydrogen 1.008	Atomic # Symbol Name Atomic Mass																2 He Helium 4.0026																													
3 Li Lithium 6.941	4 Be Beryllium 9.0122	<table border="1"> <tr> <td>C Solid</td> <td>Hg Liquid</td> <td>H Gas</td> <td>Rf Unknown</td> </tr> </table>										C Solid	Hg Liquid	H Gas	Rf Unknown	13 B Boron 10.811	14 C Carbon 12.011	15 N Nitrogen 14.007	16 O Oxygen 15.999	17 F Fluorine 18.998	18 Ne Neon 20.180																									
C Solid	Hg Liquid	H Gas	Rf Unknown																																											
11 Na Sodium 22.990	12 Mg Magnesium 24.305	<table border="1"> <tr> <td>Al Alkali metals</td> <td>Sc Alkali earth metals</td> <td>Ti Lanthanoids</td> <td>V Actinoids</td> <td>Cr Transition metals</td> <td>Mn Transition metals</td> <td>Fe Transition metals</td> <td>Co Transition metals</td> <td>Ni Transition metals</td> <td>Cu Poor metals</td> <td>Zn Poor metals</td> <td>Ga Other nonmetals</td> <td>Ge Other nonmetals</td> <td>As Other nonmetals</td> <td>Se Other nonmetals</td> <td>Br Other nonmetals</td> <td>Kr Noble gases</td> </tr> </table>										Al Alkali metals	Sc Alkali earth metals	Ti Lanthanoids	V Actinoids	Cr Transition metals	Mn Transition metals	Fe Transition metals	Co Transition metals	Ni Transition metals	Cu Poor metals	Zn Poor metals	Ga Other nonmetals	Ge Other nonmetals	As Other nonmetals	Se Other nonmetals	Br Other nonmetals	Kr Noble gases	19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
Al Alkali metals	Sc Alkali earth metals	Ti Lanthanoids	V Actinoids	Cr Transition metals	Mn Transition metals	Fe Transition metals	Co Transition metals	Ni Transition metals	Cu Poor metals	Zn Poor metals	Ga Other nonmetals	Ge Other nonmetals	As Other nonmetals	Se Other nonmetals	Br Other nonmetals	Kr Noble gases																														
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.906	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.905	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29																													
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222.2176																													
87 Fr Francium 223	88 Ra Radium 226	89-103 Actinoids	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 264	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 267	111 Rg Roentgenium 268	112 Uub Ununbium 269	113 Uut Ununtrium 270	114 Uuq Ununquadium 271	115 Uup Ununpentium 272	116 Uuh Ununhexium 273	117 Uus Ununseptium 274	118 Uuo Ununoctium 276																													

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

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57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 145	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.256	69 Tm Thulium 168.934	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.967
89 Ac Actinium 227	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237	94 Pu Plutonium 244	95 Am Americium 243	96 Cm Curium 247	97 Bk Berkelium 247	98 Cf Californium 251	99 Es Einsteinium 252	100 Fm Fermium 257	101 Md Mendelevium 258	102 No Nobelium 259	103 Lr Lawrencium 260

- Modern periodic table (PT), 118 elements, lightest H and the heaviest Uuo (Z=118)
- But have we reached the end of the PT?
- What is the heaviest element in the Periodic System?
- Are there still undiscovered ones that exist in nature?
- Is there an 8th period and how many elements will it contain? Will we accomplish g-orbital filling?



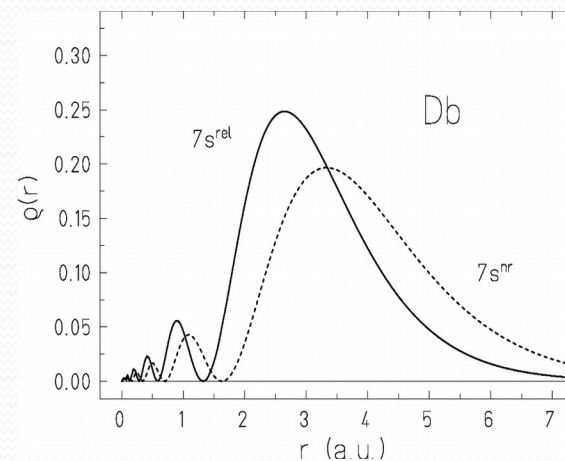
- As Z increases the electrostatic repulsion of the protons (p) cannot be sufficiently compensated by the attractive nuclear force through an increasing number of mediating neutrons (n).
- Therefore heaviest stable nuclide is $^{208}_{82}\text{Pb}$. All isotopes $Z > 82$ including some such as Bi, Th, U that are still found in nature as remnants of nucleosynthesis, are unstable, decay by α or β particle emissions, back to Pb.
- Natural ^{237}Np and natural ^{239}Pu by n capture on ^{235}U and ^{238}U respectively.
- Natural SHE, $Z=122$, $A=292$, abundance $\sim 1 \times 10^{-12}$ relative to $^{\text{nat}}\text{Th}$? Marinov et al (2010). Not validated.
- Therefore all elements $Z > 94$ (Pu) are man-made.



- From 1940 -1952: heavy elements (actinides) up till Fm synthesised in nuclear reactors by successive n capture and β^- decay and in thermonuclear explosions by rapid multiple n capture (Es, Z=99 and Fm, Z=100).
- Weighable quantities of long-lived isotopes separated. Chemical separation and identification played a crucial role. From the mid-fifties Heavy Ion (HI) fusion reactions began to be used for heavy element synthesis
- Transactinide elements ($Z \geq 103$) in present time synthesised by HI fusion reactions at high power accelerators, “one-atom-at-a-time” level with beams O to Zn. Currently $^{294}118$ heaviest known nucleus. Some theoretical estimates place $Z \sim 300$, $A \sim 960$ as the limit of the existence of the nucleus as bound entity.
- To qualify as a chemical element, the nucleus of the longest lived isotope must live $> 10^{-14}$ s, the time for the formation of an electronic shell. Many transactinide isotopes are short-lived nuclides ($T_{1/2} < 1$ s), hence physical methods of separation and identification are used.



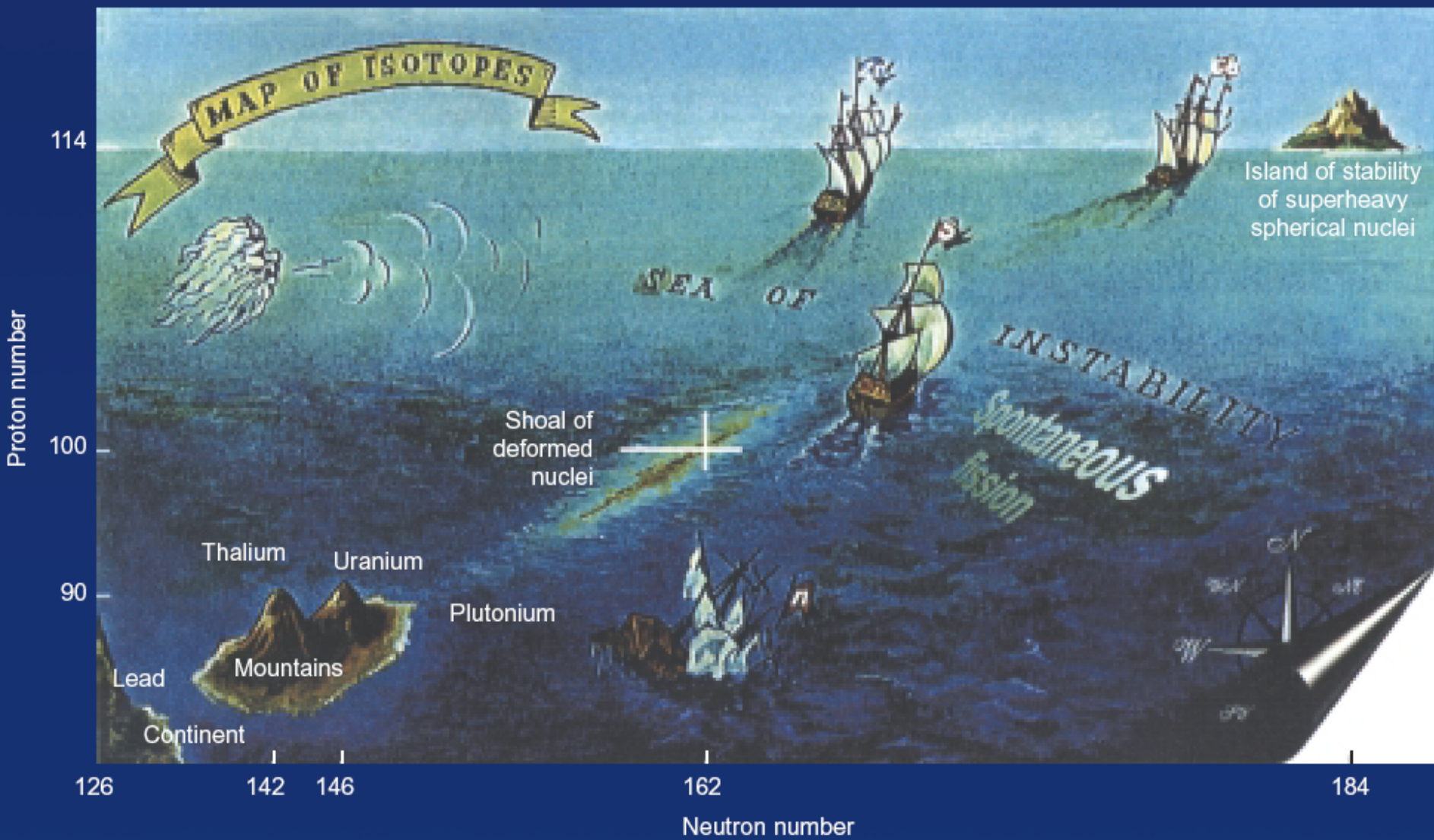
- Chemistry of the transactinides very challenging.
- Development of unique methods to isolate and determine chemical properties at the 1-3 atom level within elemental lifetimes of a few seconds! Theory plays an important role and often the only source of chemical information.
- At such high Z relativistic effects very important.
Due to stronger core attraction, the e^- moves faster causing its velocity v , mass m to relativistically increase and the radius of the ns orbitals to decrease.
- Due to higher shielding, the outer d and f orbitals expand





Shell Model

- 1949 Shell Model (Mayer and Jensen): special stability at the “magic numbers” of Z and N of 2, 8, 20, 28, 50, 82 and 126 (N only) -> Nucleons formed filled closed shells, large gap in single-particle energies to the next available shell. $^{208}_{82}\text{Pb}_{126}$ heaviest doubly magic spherical nucleus.
- The macroscopic charged liquid drop model predicts spontaneous fission (SF) barrier $B_f \sim 0$ at $Z=100$. However this model cannot explain the nearly constant $B_f \sim 6$ MeV from U -Fm. Strutinsky introduced a microscopic correction for p and n shell fillings; explained these non-zero B_f and predicted the existence of elements beyond $Z = 100$.
- Calculations (1960s) predicted the existence of a so-called island of stability (some nuclei with $T_{1/2}$ of billions of years) associated with spherical shell closures at $N = 184$ and $Z = 114$, but not $Z = 126$
- Sparked great interest in extending the periodic table out to the island by creating new elements.
- More refined theoretical calculations mutually agree on a large spherical shell gap at $N = 184$ but different approaches provide $Z = 114, 120, \text{ or } 126$ as the next spherical shell closure. They also predict large gaps in the single-particle levels at $Z = 102, 108$ and $N = 152, 162$ for deformed shapes - these regions might then have observable $T_{1/2}$.



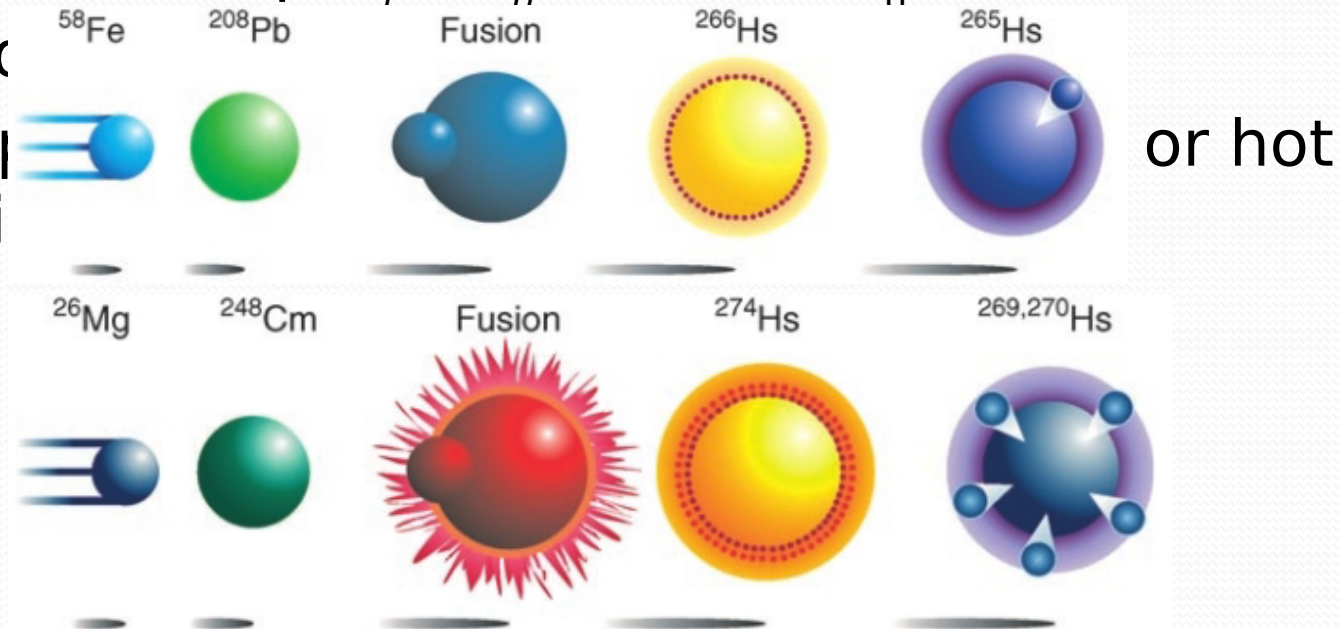


Fusion Reactions to Synthesize SHE

- The fusion evaporation residue (EVR) cross section is determined by: (cross section for the formation of an SHN as a compound nucleus (CN) with excitation energy, E^*) multiplied by (probability of its survival, $P_{xn}(E^*)$, during de-excitation by emission of x neutrons and γ -rays).

$P_{xn}(E^*) \propto \exp(B_f - B_n)$, where B_n is the neutron binding energy

- 2 approaches



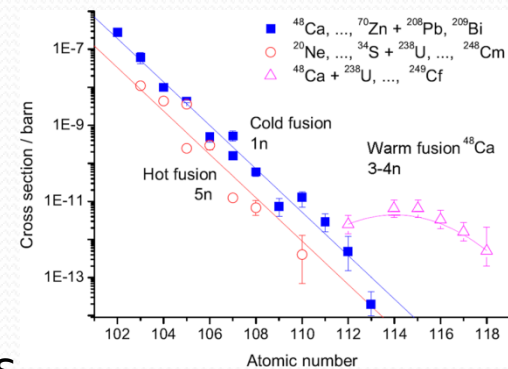


Cold fusion

- Medium-heavy stable nuclei ($A \geq 50$) bombard the spherical nuclear target ^{208}Pb or ^{209}Bi at energies just sufficient to surmount the Coulomb barrier, leaving a cold CN with $E^* \sim 10\text{-}15$ MeV.
- 1-2 n must evaporate to prevent fission of the CN.
- Transactinides $Z=107 - 112$ synthesised at GSI Darmstadt.
- But cold fusion cross sections decrease rapidly with Z_{CN} (higher coulomb barriers) and the evaporation residuals (EVRs) 10-15 mass units from the β -stability line, therefore very short-lived.

Warm fusion

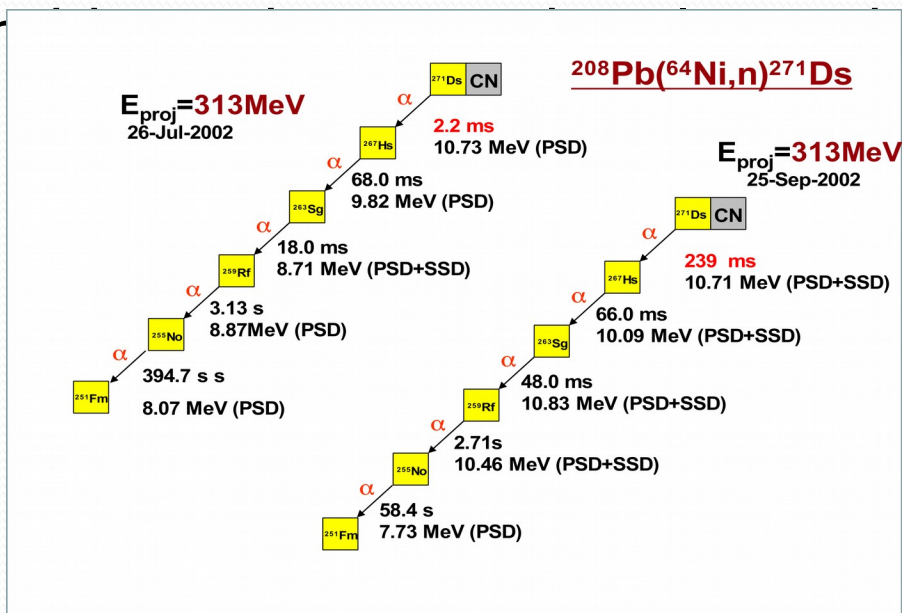
- Lower Z projectiles to reduce the Coul. barrier.
- β -stability line and new shell $N=184$ approached by n-rich target and projectile. Hence long-lived actinides e.g. ^{249}Bk as target, and doubly magic n-excess ^{48}Ca as projectile.
- $E^* \sim 30\text{-}40$ MeV, leading to 3-4 n evaporation that competes with fission for survival probability.
- But strong shell effects predicted for $Z \geq 112$, $N \geq 170$, that increase B_f , therefore increasing survival probability.
- SHE , $Z=114 -118$ synthesised at FLNR, Dubna.





Separation and Detection

- The SHE decay by a succession of α s that terminate in the SF of the ultimate decay product.
- If this last product is a well-identified nucleus the identity of the progenitors is secured by the number of α decays in the genetic chain (each decay takes away $Z=2$ and $N=2$).
- Unique identification becomes more difficult if the decays are in the uncharted region.



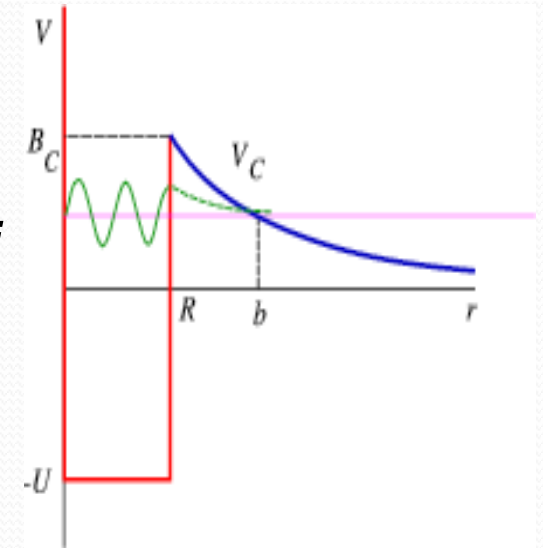


Alpha decay - dominant decay mode of heavy EVR formed in HI-fusion reactions in the synthesis of SHE.

Successive α decays terminate in spontaneous fission form a genetic chain that help to identify the SHEs.

Experimental identification of the short-lived isotopes aided by theoretical predictions of the half-lives and decay energies. An *a priori* knowledge of the half-life essential to the nuclear chemist for the design and execution of the chemical properties of the SHE.

α Decay Mechanism: QM tunnelling through the potential energy (PE) barrier. Net energetics as Q_α . Barrier penetrability e.g. WKB calculation, α decay constant $\lambda_\alpha = \ln 2 / T_\alpha$



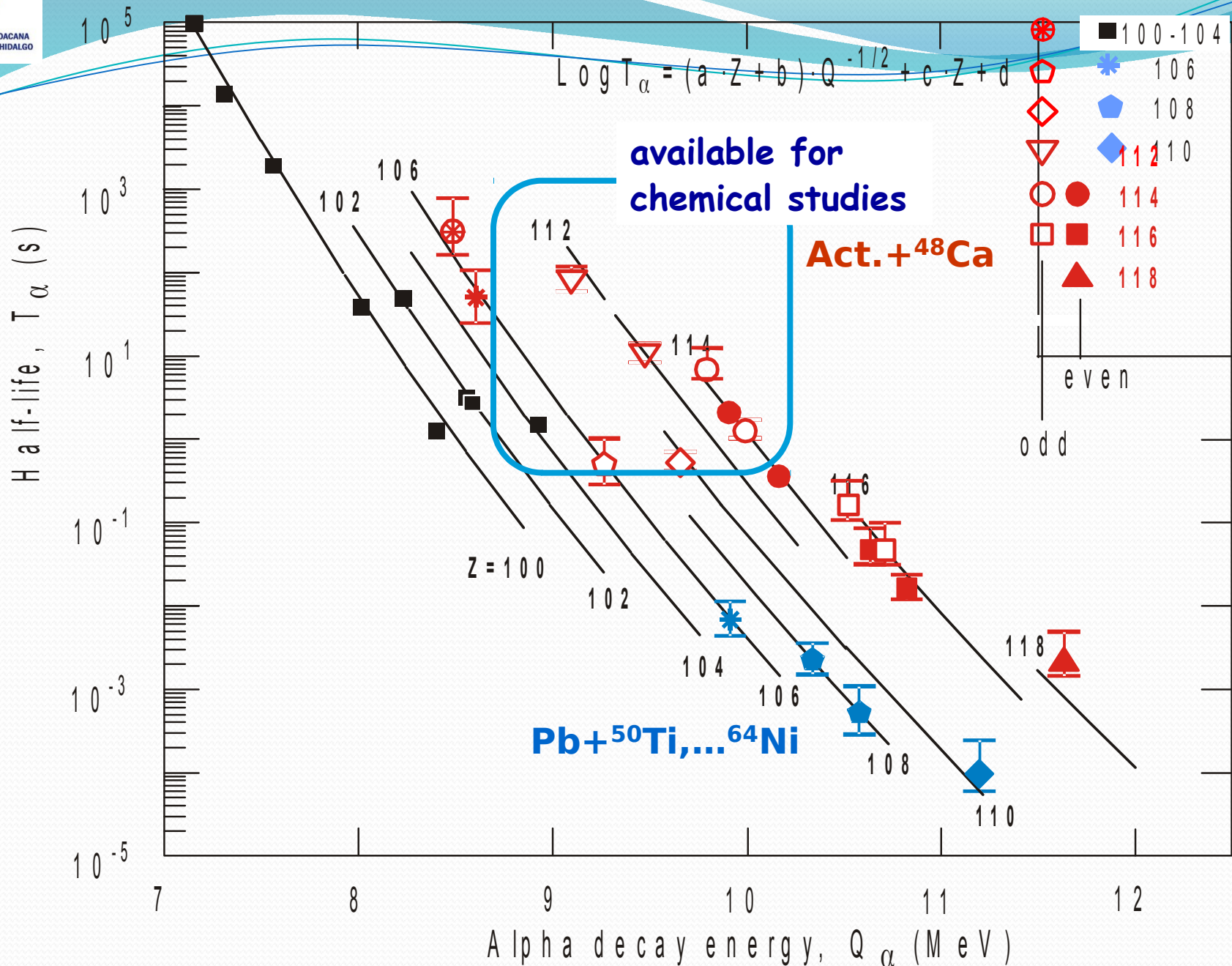


Several microscopic models. Some macroscopic models such as the Generalised Liquid Drop Model (GLDM) and the Supersymmetric Fission Model as well as phenomenological observations have been reduced to analytical formulae.

Advantages of analytical formulae: rapid prediction of T_α for the observation of systematics over wide Z,A region; facile upgrade of coefficients with the expansion/refinement of experimental data; easy incorporation into data acquisition and analysis softwares requiring fewer cpu/memory resources.

A well-established formula aids the identification and characterization of the SHE. Predictive accuracy of a chosen formula must be established to ascertain its reliability in the prediction of T_α for newly discovered α emitters.

Oganessian et al at Dubna use the Viola-Seaborg, Andreas Tuerler et al at Darmstadt favour the Sobiczewski formula (ENAM 2008 personal comm..) ; Ken Moody of LBL uses the Geiger-Nuttal systematics (NP A734 (2004) 188)





Extant works:

- Compare the predicted T_α with the experimental T_α of SHE.
 - Does not permit a sufficiently conclusive statistical evaluation - insufficient basis set (too few well characterized SHE)
 - Cyclic argument
- Basis set contains nuclides far from the line of β stability: uncertain alpha spectrometric data such as the α branching fractions (e.g. $^{110,111}\text{Xe}$, ^{111}I , ^{180}Bi).
 Q_α are only known from systematics.

Such inclusions cause slight variations in the coefficient values : effect of T_α amplified because of the logarithmic relationship.



- Consequently, it becomes difficult to compare the predictive abilities of each formula, and hence the degree of reliability when applied to completely unknown nuclides.
- Analogous to the testing of reliability of any experimental procedure / instrument.
- Indeed in the context of SHE synthesis, α decay formulae function as probe “instruments” hand-in-hand with α spectrometers.
- Standard experimental validation procedure (IUPAC Guideline for validation of methods of analysis by Thompson et al, Pure Appl. Chem., 74(5), pp. 835-55, 2002):
 - 1) Calibration of method using absolute standards.
 - 2) Validating method using certified reference materials – “Fitness of purpose”
 - 3) Pronouncing the reliability in terms of the figures of merit (Trueness or Relative error and Precision)



In this work:

we devise a method based on the *ansatz* of standard experimental benchmarking (the IUPAC guideline), to,

- **systematically investigate the reliability of the 3 most commonly used formulae, the Viola-Seaborg, the Sobiczewski-Parkhomenko and Royer's GLDM formula**

and to

- **check the predictive accuracy of our modified formulae for the T_{α} of SHE and nuclei near the p drip-line - collectively, EXOTIC nuclei**



- **GLDM formula of Royer (R)**

α decay as a quasi-molecular path within the GLDM including proximity effects between nucleons in the neck and shell effects given by the droplet model. T_α deduced using the WKB for spontaneous asymmetric fission.

$$\log_{10}[T_\alpha(\mathbf{R})] = \mathbf{a} + \mathbf{b} \cdot \mathbf{A}^{1/6} \cdot \mathbf{Z}^{1/2} + \mathbf{c} \cdot \mathbf{Z} / (\mathbf{Q}_\alpha)^{1/2}$$

$T_\alpha(\mathbf{R})$ is the calculated alpha partial half-life (s); Q_α in MeV.

- **Viola-Seaborg formula (VS)**

In 1966 Viola and Seaborg generalised the empirical Geiger-Nuttall formula to obtain a 7 parameter formula for the partial half-life, $T_\alpha(\text{VSS})$.

$$\log_{10}[T_\alpha(\text{VSS})] = (\mathbf{a} \cdot \mathbf{Z} + \mathbf{b}) \cdot (\mathbf{Q}_\alpha)^{-1/2} + (\mathbf{c} \cdot \mathbf{Z} + \mathbf{d}) + \mathbf{h}_{\log}$$

h_{\log} is the hindrance factor for nuclei with unpaired nucleons. It is obtained by fits to odd nuclei.

- **Sobiczewski-Parkhomenko formula (SP)**

In 2005 S and P introduced a 5 parameter phenomenological formula that simplifies the VS formula

$$\log_{10}[T_\alpha(\text{SP})] = \mathbf{a} \cdot \mathbf{Z} \cdot (\mathbf{Q}_\alpha - \bar{\mathbf{E}}_i)^{-1/2} + \mathbf{b} \cdot \mathbf{Z} + \mathbf{c}$$

$\bar{\mathbf{E}}_i$ is the average excitation energy of a state of the daughter nucleus to which the α decay goes.



Method

We devise a calibration and validation protocol analogous to the IUPAC guideline : The analytical formula is treated as an “instrument” of the experiment, which is calibrated and then probed for systematic and random errors.

- A fixed sized basis set with very well characterized α spectroscopic and mass data – the set of reference nuclei (REF) - is chosen to derive anew the coefficients of all 3 formulae. This step defines “calibration” (IUPAC guideline).
- A larger set of nuclides (TEST) of well-known mass and α data are used to validate the calibrated formulae . “Fitness of purpose” (IUPAC guideline).

Some adjustments to calibrated formulae made to improve the statistics.

Predictability of the 3 formulae stated in terms of the statistical FOMs

- The validated formulae used to obtain the $T\alpha$ of Exotic α emitters.

REF set:

- 78 α energy and intensity standards (Firestone & Shirley, Table of Isotopes, 8th Edn, 1998).
- Medium-sized basis set such that the resulting modified formulae (suffix “m”) are not expected to produce close agreements between T_{α}^{calc} and T_{α}^{exp} for nuclei far outside its range.

However that is not the main intention of the present work. The intention is to produce formulae with highly reliable coefficients that can be used to test the predictability of the m-formulae using an independent and approximately similar data set (the TEST set).

TEST set:

- 235 experimentally well-characterized α emitters with a (Z,N) range close to the REF to reduce the possibility of the influence of (Z,A) dependent differences in the underlying nuclear parameters, in the data analysis.

REF and TEST are the analogues of the “calibration standard” and “standard reference material” in experimental practice.



- EXOTIC set – 96 α emitters, from medium-mass to SHE.
- The standard Levenberg-Marquardt non-linear multivariate regression fitting algorithm (*Mathematica* 5.2) was used to derive the coefficient values and their errors using the spectroscopic errors of the REF set

VS and SP formulae: In variant m1 all parameters except h_{\log} and \bar{E}_i determined from the even-even parity sets, whereas in m2 the parameters are determined separately for each parity set.



- Figure of Merit for accuracy is taken as the Relative Error (IUPAC, 2002), RE

$$RE = \left| \left[\log_{10}(T_{\alpha})^{\text{exp}} - \log_{10}(T_{\alpha})^{\text{calc}} \right] / \log_{10}(T_{\alpha})^{\text{exp}} \right|$$

$$\text{Accuracy Index} = 1 - RE$$

- Following Sobieczewski and Parkhomenko, the index f is a valid FOM . It is a function of the average discrepancy δ_{av} that determines the average multiplicative factor of $(T_{\alpha})^{\text{calc}}$ over $(T_{\alpha})^{\text{exp}}$

$$\delta_{av} = (1/N) \sum_{i=1}^N \left[\log_{10}(T_{\alpha})^{\text{calc}} / \log_{10}(T_{\alpha})^{\text{exp}} \right]$$

$$f = 10^{\delta}$$



Results and Discussion

Coefficients of the modified Royer's GLDM formula (Rm), modified Viola-Seaborg formula (VSm1 and VSm2) and the modified Sobiczewski-Parkhomenko formula (SPm1 and SPm2) calculated from the REF set. For the e-e sub-set, m1 and m2 are the same. RMSRE is the rms value of the RE

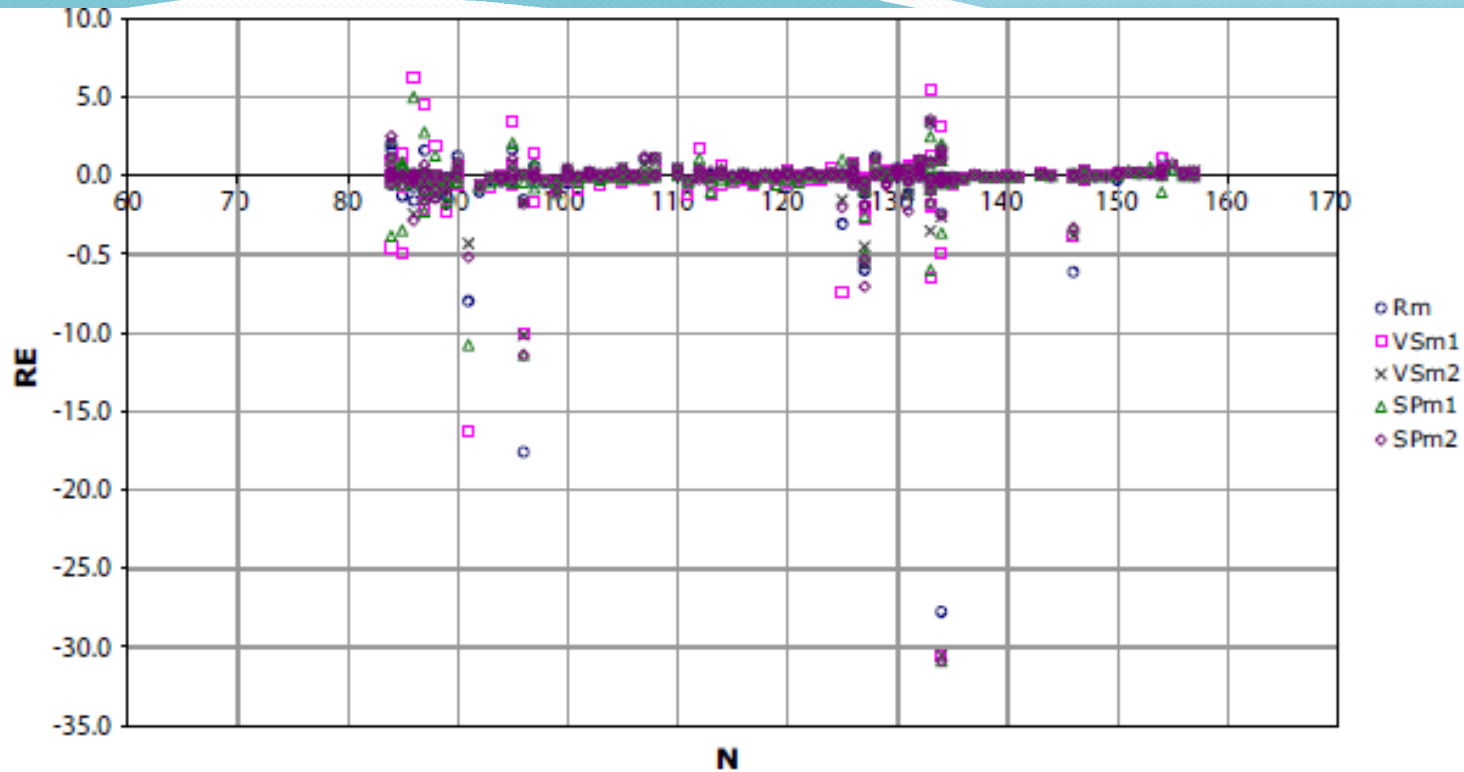
Formula	Z, N	Coefficients						RMSRE
		a	b	c	d	h_{log}	E_i	
Rm	e-e	-22.2505 ±0.2465	-1.191 ±0.013	1.5226 ±0.0018	-	-	-	0.0434
	e-o	-27.773 ±0.2833	-1.0032 ±0.0045	1.5809 ±0.0041	-	-	-	0.0733
	o-e	-29.2562 ±0.4892	-1.0279 ±0.0077	1.6198 ±0.0070	-	-	-	0.0546
	o-o	-28.3003 ±0.0528	-1.3553 ±0.0161	1.8264 ±0.0101	-	-	-	0.1899
VSm1	e-e	1.4833 ±0.0115	2.0678 ±1.1487	-0.2107 ±0.0045	-30.533 ±0.4533	0.0	-	0.0469
	e-o	1.4833 ±0.0115	2.0678 ±1.1487	-0.2107 ±0.0045	-30.533 ±0.4533	1.2023 ±0.0177	-	0.0775
	o-e	1.4833 ±0.0115	2.0678 ±1.1487	-0.2107 ±0.0045	-30.533 ±0.4533	0.6650 ±0.0285	-	0.0656
	o-o	1.4833 ±0.0115	2.0678 ±1.1487	-0.2107 ±0.0045	-30.533 ±0.4533	1.1044 ±0.0968	-	0.2380
VSm2	e-e	1.4833 ±0.0115	2.0678 ±1.1487	-0.2107 ±0.0045	-30.533 ±0.4533	-	-	(0.0469)
	e-o	1.5206 ±0.0069	4.3178 ±0.2335	-0.1613 ±0.0006	-36.2658 ±0.1264	-	-	0.0737
	o-e	1.6077 ±0.0433	-0.8714 ±3.5349	-0.1987 ±0.0190	-34.5795 ±1.5382	-	-	0.0552
	o-o	3.0915 ±0.0103	-108.543 ±1.6435	-0.8145 ±0.0056	11.3339 ±0.7473	-	-	0.1415
SPm1	e-e	1.5066 ±0.0015	-0.2231 ±0.0024	-29.4184 ±0.1656	-	-	0.0	0.0473
	e-o	1.5066 ±0.0015	-0.2231 ±0.0024	-29.4184 ±0.1656	-	-	0.1609 ±0.0027	0.0925
	o-e	1.5066 ±0.0015	-0.2231 ±0.0024	-29.4184 ±0.1656	-	-	0.1048 ±0.0053	0.0705
	o-o	1.5066 ±0.0015	-0.2231 ±0.0024	-29.4184 ±0.1656	-	-	0.2657 ±0.0059	0.2504
SPm2	e-e	1.5066 ±0.0015	-0.2231 ±0.0024	-29.4184 ±0.1656	-	-	0.0	(0.0473)
	e-o	1.549 ±0.0012	-0.1796 ±0.0020	-34.095 ±0.2797	-	-	0.0441 ±0.0059	0.0733
	o-e	1.5892 ±0.0478	-0.1897 ±0.0147	-35.2072 ±0.0318	-	-	0.0246 ±0.0993	0.0552
	o-o	10.8468 ±0.6325	-1.9971 ±0.0924	-33.9546 ±0.0531	-	-	-13.4983 ±0.8191	0.1378



- The RMSRE with its standard deviation, RMS[s(RE)], the f values and the t statistics at 90% and 95% confidence level of the modified formulae applied to the TEST nuclides.
- VSm2 and SPm2 better than their m1 counterparts.
- The few number of REF o-o nuclei cause the o-o subset to have the poorest FOMs.
- RM and VSm2 tied as the best prescriptions.

Formula	Z, N	RMSRE±RMS[s(RE)]	Avg. RMSRE	\bar{f}	Avg. \bar{f}
Rm	e-e	3.812 ± 2.084	1.745 ± 0.591	2.510	4.088
	e-o	1.434 ± 1.001		4.100	
	o-e	0.693 ± 0.484		3.870	
	o-o	1.039 ± 0.106		5.873	
VSm1	e-e	3.681 ± 1.671	2.247 ± 0.717	2.358	7.570
	e-o	2.593 ± 2.071		12.00	
	o-e	1.410 ± 0.894		6.160	
	o-o	1.302 ± 0.594		9.765	
VSm2	e-e	(3.681 ± 1.671)	1.638 ± 0.456	(2.358)	4.440
	e-o	1.036 ± 0.545		3.328	
	o-e	0.753 ± 0.357		3.990	
	o-o	1.081 ± 0.321		8.082	
SPm1	e-e	3.763 ± 1.978	1.950 ± 0.626	2.448	5.600
	e-o	1.675 ± 1.260		5.794	
	o-e	1.106 ± 0.682		4.570	
	o-o	1.257 ± 0.546		9.589	
SPm2	e-e	(3.763 ± 1.978)	1.775 ± 0.556	(2.448)	9.352
	e-o	1.106 ± 0.905		3.588	
	o-e	0.805 ± 0.435		4.120	
	o-o	1.426 ± 0.167		27.25	

Formula pairs	Z, N	t	t_{90}	t_{95}
VSm2 vs. VSm1	e-o	5.906	< 1.660	< 1.984
	o-e	5.057	< 1.660	< 1.984
	o-o	1.968	< 1.667	< 1.994
SPm2 vs. SPm1	e-o	2.980	< 1.660	< 1.984
	o-e	2.762	< 1.660	< 1.984
	o-o	1.777	< 1.667	< 1.994



- Plot of the variation of the relative error (RE) between calculated and experimental T_α w.r.t neutron number (N) for the TEST set.
- Most RE are small but large deviations near the shell closure numbers of 82, 126 and N=146 (“deformed magic”), also around N = 88-90 (“shape transition”), N= 96-98 (“loss of collectivity and sub-shell gaps”) and N= 134 (“static octupole deformation”).



- 46 e-e alpha decays of the EXOTIC set calculated by the modified formulae with the corresponding experimental values . The complete data for all parity types are to be found in Dasgupta-Schubert and Reyes At. Data Nucl. Data Tables 93(2007) 907 and Dasgupta-Schubert et al, Europhys. Journal A, 42 (2009) 121.
- The synthesis of SHE and nuclides near the p drip-lines require accurate theoretical mass estimates to get the predicted Q_α and hence the T_α . We have used the Finite Range Droplet Model (FRDM) of nuclear masses (Dasgupta-Schubert and Reyes, ADNDT 93(2007) 907) and have shown that the Rm formula that results must be used self-consistently i.e. always with the FRDM masses for reasonable accuracy in the predictability.

Even-even parent									
Parent	Z	A	Q_α^{exp} (MeV)	T_α^{exp} (s)	$\log_{10} T_\alpha^{\text{exp}}$ (s)	$\log_{10} T_\alpha^{\text{calc}}$ (s)			
						Rm	VSm2	SPm2	
Er	68	156	3.49	2.30E10 ± 1.2E+08	10.36	10.42 ± 0.06	10.27 ± 0.05	10.28 ± 0.06	
Yb	70	158	4.17	4.30E06 ± 3.75E05	6.63	6.76 ± 0.05	6.57 ± 0.03	6.60 ± 0.05	
W	74	158	6.61 ± 0.00	1.50E-03 ± 2.00E-03	-2.82	-2.25 ± 0.04	-2.63 ± 0.00	-2.57 ± 0.03	
Os	76	162	6.80 ± 0.00	1.90E-03 ± 2.00E-03	-2.72	-2.11 ± 0.03	-2.51 ± 0.00	-2.45 ± 0.03	
Os	76	164	6.48	4.20E-02 ± 2.00E-03	-1.38	-1.07 ± 0.03	-1.43 ± 0.00	-1.37 ± 0.03	
Pt	78	166	7.29	3.00E-04	-3.52	-2.91 ± 0.03	-3.34 ± 0.01	-3.28 ± 0.02	
Pt	78	168	7.00	2.00E-03 ± 4.00E-04	-2.70	-2.06 ± 0.03	-2.44 ± 0.00	-2.39 ± 0.03	
Pt	78	170	6.71	1.40E-02 ± 1.17E-02	-1.85	-1.15 ± 0.03	-1.50 ± 0.00	-1.45 ± 0.03	
Hg	80	172	7.53	4.20E-04	-3.38	-2.97 ± 0.02	-3.37 ± 0.01	-3.33 ± 0.02	
Hg	80	174	7.23	2.10E-03	-2.68	-2.13 ± 0.02	-2.49 ± 0.01	-2.45 ± 0.02	
Pb	82	178	7.79	2.30E-04	-3.63	-3.10 ± 0.02	-3.49 ± 0.01	-3.45 ± 0.02	
Pb	82	180	7.42	5.00E-03	-2.30	-2.03 ± 0.02	-2.38 ± 0.01	-2.34 ± 0.02	
Pb	82	184	6.77	6.10E-01 ± 6.65E-02	-0.22	0.00 ± 0.02	-0.28 ± 0.00	-0.25 ± 0.02	
Pb	82	186	6.47	1.20E+01 ± 1.24E-01	1.08	1.07 ± 0.02	0.82 ± 0.00	0.86 ± 0.02	
Pb	82	194	4.74	9.80E+09 ± 4.08E+08	9.99	9.16 ± 0.03	9.02 ± 0.01	9.05 ± 0.03	
Po	84	188	8.09 ± 0.025	4.00E-04 ± 2.00E-04	-3.40	-3.40 ± 0.01	-3.69 ± 0.01	-3.66 ± 0.01	
Po	84	190	7.69	2.50E-03 ± 6.25E-04	-2.60	-2.31 ± 0.01	-2.56 ± 0.01	-2.53 ± 0.01	
Po	84	192	7.32 ± 0.011	2.90E-02 ± 1.50E-02	-1.54	-1.19 ± 0.02	-1.41 ± 0.00	-1.38 ± 0.01	
Po	84	194	6.99 ± 0.003	4.215E-01 ± 4.30E-03	-0.38	-0.13 ± 0.02	-0.31 ± 0.00	-0.28 ± 0.01	
Rn	86	196	7.62 ± 0.009	4.40E-03 ± 1.30E-03	-2.36	-1.42 ± 0.01	-1.68 ± 0.00	-1.65 ± 0.01	
Rn	86	198	7.35	6.50E-02 ± 2.03E-03	-1.19	-0.61 ± 0.01	-0.83 ± 0.00	-0.81 ± 0.01	
Ra	88	202	8.02	2.60E-03 ± 1.23E-02	-2.59	-2.00 ± 0.01	-2.25 ± 0.01	-2.23 ± 0.00	
Ra	88	204	7.64	5.90E-02 ± 1.20E-02	-1.23	-0.87 ± 0.01	-1.09 ± 0.00	-1.07 ± 0.01	
Th	90	210	8.05 ± 0.02	9.00E-03 ± 1.15E-02	-2.05	-1.51 ± 0.00	-1.72 ± 0.01	-1.71 ± 0.00	
U	92	218	8.77 ± 0.01	5.10E-04 ± 1.70E-04	-3.29	-2.98 ± -0.01	-3.14 ± 0.01	-3.15 ± 0.01	
U	92	220	10.30	6.00E-08	-7.22	-6.67 ± -0.01	-6.75 ± 0.01	-6.75 ± 0.01	
U	92	224	8.62	7.00E-04 ± 2.3E-10	-3.16	-2.69 ± -0.01	-2.73 ± 0.01	-2.73 ± 0.01	
Pu	94	228	7.95	2.00E-01	-0.700	-0.03 ± -0.01	-0.15 ± 0.00	-0.16 ± 0.01	
Pu	94	230	7.18	1.00E+02	2.00	2.58 ± 0.00	2.47 ± 0.00	2.46 ± 0.01	
Cm	96	238	6.62	2.30E+05 ± 9.58E+03	5.36	5.51 ± -0.01	5.39 ± 0.00	5.38 ± 0.01	
Fm	100	250	7.56 ± 0.01	2.00E+03 ± 2.00E+02	3.30	3.24 ± -0.02	3.11 ± 0.00	3.08 ± 0.02	
No	102	258	8.15	1.20E+02	2.08	1.80 ± -0.02	1.70 ± 0.00	1.65 ± 0.02	
Rf	104	256	8.95	3.04E-01	-0.52	0.07 ± -0.03	-0.19 ± 0.00	-0.25 ± 0.03	
Rf	104	258	9.25	9.20E-02 ± 1.53E-02	-1.04	-0.83 ± -0.03	-1.04 ± 0.00	-1.10 ± 0.03	
Rf	104	260	8.901	1.00E+00 ± 3.48E-02	0.00	0.14 ± -0.03	-0.04 ± 0.00	-0.10 ± 0.03	
Sg	106	260	9.92	7.20E-03	-2.14	-1.99 ± -0.03	-2.29 ± 0.01	-2.36 ± 0.04	
Hs	108	264	10.8	8.1E-05	-4.09	-3.56 ± -0.04	-3.91 ± 0.01	-4.00 ± 0.04	
Hs	108	266	10.34	2.30E-03	-2.64	-2.50 ± -0.04	-2.82 ± 0.01	-2.91 ± 0.04	
Hs	108	270	9.02	2.20E+01	1.34	1.04 ± -0.03	0.74 ± 0.01	0.67 ± 0.04	

Even-even parent									
Parent	Z	A	Q_α^{exp} (MeV)	T_α^{exp} (s)	$\log_{10} T_\alpha^{\text{exp}}$ (s)	$\log_{10} T_\alpha^{\text{calc}}$ (s)			
						Rm	VSm2	SPm2	
Ds	110	270	11.20	1.00E-04	-4.00	-3.96 ± -0.04	-4.33 ± 0.01	-4.44 ± 0.05	
Ds*						(-3.96 ± 0.13)*	(-4.33 ± 0.08)*	(-4.44 ± 0.14)*	
Uuq	114	286	10.35 ± 0.06	1.60E-01 ± 7.00E-02	-0.80	-0.94 ± -0.05	-1.34 ± 0.01	-1.46 ± 0.05	
Uuq	114	288	10.09 ± 0.07	8.00E-01 ± 3.20E-01	-0.10	-0.28 ± -0.05	-0.66 ± 0.01	-0.78 ± 0.05	
Uuh	116	290	11.00 ± 0.08	1.50E-02 ± 2.60E-02	-1.82	-2.00 ± -0.05	-2.47 ± 0.02	-2.60 ± 0.06	
Uuh	116	292	10.80 ± 0.07	1.80E-02 ± 1.60E-02	-1.75	-1.55 ± -0.05	-1.98 ± 0.02	-2.12 ± 0.06	
Uuo	118	294	11.81 ± 0.06	1.80E-03 ± 7.50E-02	-2.75	-3.33 ± -0.06	-3.86 ± 0.02	-4.01 ± 0.06	



- The small statistics of the odd parity sets of REF (particularly the o-o) cause a statistical disadvantage to the coefficients of the modified formulae.
- A *pseudo* increase of the statistics is attempted by linearly fitting the $\log_{10}(T_{\alpha})^{\text{calc}}$ obtained from the modified formulae with the $\log_{10}(T_{\alpha})^{\text{exp}}$ of the TEST set to yield the linearly optimised log of the calculated T_{α} , $\log_{10}(T_{\alpha}^{\text{lin-opt}})$. The regression equation is

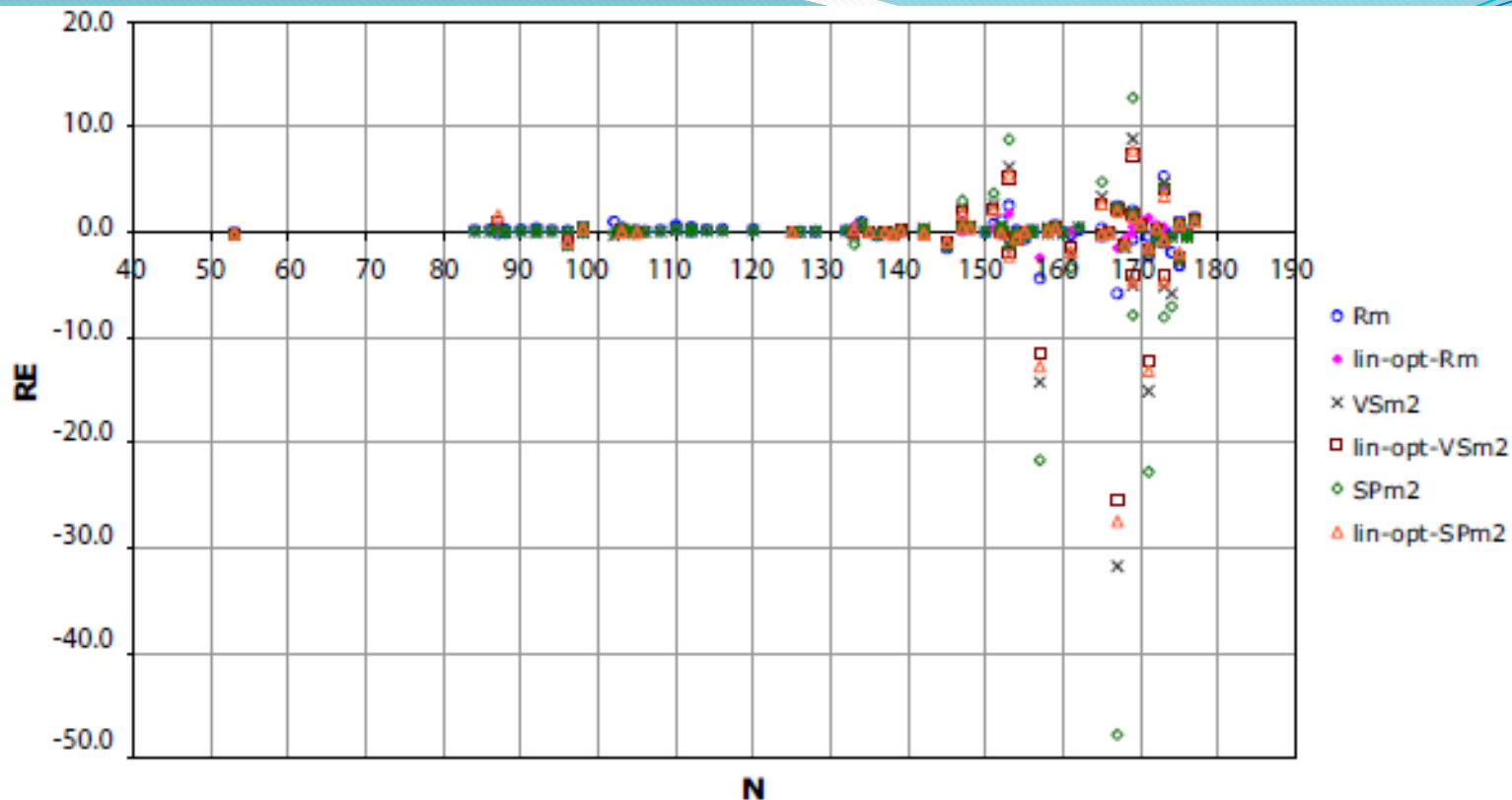
$$\log_{10}(T_{\alpha}^{\text{lin-opt}}) = \mu \cdot \log_{10}(T_{\alpha})^{\text{calc}} + \kappa$$

The RMSRE and its average value for the original and the modified formulae including the linearly optimised variant for the o-o subset, for the EXOTIC nuclei.

- Linear optimization improves the accuracy of the o-o subset. The accuracies for the modified formulae are lower than the original formulae. When the o-o set is excluded, RMSRE of the modified and original formulae are close, the ratios being ≤ 1.2 . Hence despite the lowered statistics and the much lower (Z,A) range of the REF as well as the non-exclusion of nuclei near N shell closures, the modified formulae perform well.

- Overall, Rm yields the best results. VS and SP involve straight utilization of Geiger Nuttall

Formula	Z, N	RMSRE ^a	Avg. RMSRE (all parities)	Avg. RMSRE (odd parities)
R	e-e	0.391	0.761	0.884
	e-o	1.137		
	o-e	0.573		
	o-o	0.943		
Rm	e-e	0.448	1.209	1.462
	e-o	1.841		
	o-e	0.539		
	o-o	2.006		
Lin-opt-Rm	e-o	1.518	-	0.994
	o-e	0.502		
	o-o	0.961		
VSS	e-e	1.018	1.047	1.056
	e-o	1.468		
	o-e	0.589		
	o-o	1.113		
VSm2	e-e	0.915	3.330	4.134
	e-o	1.674		
	o-e	0.630		
	o-o	10.099		
Lin-opt-VSm2	e-o	1.485	-	3.378
	o-e	0.509		
	o-o	8.141		
SP	e-e	1.108	1.038	1.014
	e-o	1.296		
	o-e	0.693		
	o-o	1.054		
SPm2	e-e	1.094	4.613	5.786
	e-o	1.547		
	o-e	0.624		
	o-o	15.187		
Lin-opt-SPm2	e-o	1.331	-	3.550
	o-e	0.503		
	o-o	8.816		



Plot of the RE between $\log_{10}(I_{\alpha})^{\text{calc}}$ obtained from the modified and linearly optimised formulae and $\log_{10}(T_{\alpha})^{\text{exp}}$ w.r.t N for the EXOTIC set. Large deviations near the sub-shells around $N = 152, 162, 172$. Linear optimization reduces these deviations somewhat but their signatures remain. None of the 3 formulae consider shell effects directly, only indirectly via the Q_{α} .



Conclusion

- We show that the *ansatz* of experimental benchmarking can be carried over to analytical prescriptions of alpha decay half-lives, to characterize their utility as predictive tools.
- Although it has been demonstrated only for the analytical formulae, it is universal in scope and can be applied to any bank of data generated by theory.
- Indeed a knowledge of the predictability allows a judicious choice of the appropriate analytical prescription in the context of SHE synthesis and chemical characterization.
- Additionally we show that the statistical limitation of a small albeit highly reliable basis set to derive the coefficients, can be reduced by a simple local linear optimization that requires no re-tooling of the original formula.
- The modified formulae are reasonably accurate except near shell/sub-shell closures.



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heavy element region by Hyde et al. (1964).
Recently Dasgupta-Schubert and Reyes (2007) proposed a new generalized liquid-drop α -decay formula, which was based on experimental data of 373 α -emitting nuclei. According to this formula

$$\log_{10}(T_{1/2}[s]) = a + bA^{1/6}\sqrt{Z} + \frac{cZ}{\sqrt{Q_\alpha}},$$

where $T_{1/2}[s]$ is the alpha partial half-life in seconds, Z , A are the atomic and mass numbers of the mother nucleus, Q_α is the energy of α -decay, a , b , c are constants, which depend on the type of the mother nucleus:

Z	N	a	b	c
Even	Even	-25.31	-1.1629	1.5864
Even	Odd	-26.65	-1.0859	1.5848
Odd	Even	-25.68	-1.1423	1.592
Odd	Odd	-29.48	-1.113	1.6971

Handbook of Nuclear Chemistry, 2nd Edn. A. Vertes et al (Eds.), Springer, Berlin, 2011.

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