Workshop on
NUCLEAR STRUCTURE AND DECAY DATA EVALUATION

Trieste, February 18 – March 3, 2006

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Decay Data

1. Statistical treatment of data
2. Properties of the parent nucleus
3. Gamma rays
4. Decay scheme normalization
5. Beta particles
6. Electron capture
7. Alpha particles
8. Level structure and decay scheme

1. Statistical treatment of data

- Weighted and unweighted averages
- Limits
- Discrepant data
- Limitation of relative statistical weight method

2. **Properties of the parent nucleus**

- Energy, spin/parity, half-life, Q-value

3. Gamma rays

- Energy (E_γ)
- Relative intensity (I_γ)
- Multipolarity and mixing ratio (δ)
- Internal conversion coefficient (α_i)
- Total transition intensity [I_γ (1 + α)]
- Absolute intensity (%I_γ)

4. Beta particles

- Relative intensity (I_β), absolute intensity ($\%I_\beta$)
- Average energy (I_{avg})
- Log *ft*
- Energy (E_β)

5. Electron capture

- Relative probability (I_ε), absolute probability ($\%I_\varepsilon$)
- Relative sub-shell probabilities (P_K, P_L, P_M, P_N)
- Log *ft*

6. Alpha particles

- Energy (E_α)
- Relative intensity (I_α), absolute intensity ($\%I_\alpha$)
- Hindrance factor (HF)

7. Level structure and decay scheme

- Level energy (E)
- Level spin/parity (Jπ), particle configuration (CONF)
- Level half-life ($T_{1/2}$)
- Decay scheme normalization

1. Statistical treatment of data

- Average, Weighted Average (weight = $1/\sigma_i^2$)
- Limits (given by authors: <10; changed by evaluator: 5 *5*)
- Confidence level for limits deduced by evaluators from transition intensity balances (Tom Burrows will talk about this matter.)
- Discrepant data – Limitation of Relative Statistical Weight (LWEIGHT)

Averages

Unweighted

$x(avg) = 1 / n \sum x_i$

$\sigma_{x(avg)} = [\, 1 / n\,(n-1) \sum (x(avg) - x_i)^2]^{1/2}$ Std. dev.

Weighted

$x(avg) = W \sum x_i / \sigma_{xi}^2$; $W = 1 / \sum \sigma_{xi}^{-2}$

$\chi^2 = \sum (x(avg) - x_i)^2 / \sigma_{xi}^2$ Chi sqr.

$\chi_\nu^2 = 1 / (n-1) \sum (x(avg) - x_i)^2 / \sigma_{xi}^2$ Red. Chi sqr

$\sigma_{x(avg)}$ = larger of $W^{1/2}$ and $W^{1/2} \chi_\nu$. Std. dev.

Limits

B_m = measured value

σ = Standard deviation

B_0 = True value

Example: -2 ± 3

For a Gaussian distribution the formulas to convert measured values to limits are:

$B_0 < B_m + 1.28\,\sigma$ (90% confidence limit); Example: < 1.84

$B_0 < B_m + 1.64\,\sigma$ (95% confidence limit); Example: < 2.92

$B_0 < B_m + 2.33\,\sigma$ (99% confidence limit); Example; < 4.99

Discrepant Data

Simple definition: A set of data for which $\chi_\nu^2 > 1$.

But, χ_ν^2 has a Gaussian distribution, i.e. it varies with the degrees of freedom (*n – 1*).

Better definition: A set of data is discrepant if χ_ν^2 is greater than χ_ν^2 (critical). Where χ_ν^2 (critical) is such that there is a 99% probability that the set of data is discrepant.

Limitation of Relative Statistical Weight Method

For discrepant data ($\chi^2_\nu > \chi^2_\nu$(critical)) with at least three sets of input values, we apply the *Limitation of Relative Statistical Weight* method. The program identifies any measurement that has a relative weight >50% and increases its uncertainty to reduce the weight to 50%. Then it recalculates χ^2_ν and produces a new average and a best value as follows:

If $\chi^2_\nu \leq \chi^2_\nu$(critical), the program chooses the weighted average and its uncertainty (the larger of the internal and external values).

If $\chi^2_\nu > \chi^2_\nu$(critical), the program chooses either the weighted or the unweighted average, depending on whether the uncertainties in the average values make them overlap with each other. If that is so, it chooses the weighted average and its (internal or external) uncertainty. Otherwise, the program chooses the unweighted average. In either case, it may expand the uncertainty to cover the most precise input value

2. Properties of the parent nucleus

- Level energy (keV): 0.0, 328.0 *25*, 942 *4*, 0.0 + X
- Spin/parity: 1/2+, (3/2+), 5-, 6(+), (5/2-,7/2-)
- Half-life: 3.8 d *2*, 432.2 y *7*, 2 m, 35 ms *10*, ~3 s, 1.2×10^{15} y
- Units: (sidereal) y (= 365.25636 d), d, h, m, s, ms, ms, ns, ps, fs, …
- Q-value (keV): 2003Au03 (G. Audi et al., Nucl. Phys. **A729**, 337 (2003))
- Theoretical values: 1997Mo25 (P. Moller et al., At. Nucl. Data Tables **66**, 131 (1997))

3. Gamma rays

1. Energy (keV)

- Weighted average from radioactive decay
- Very precise measurements (e.g. bent crystal)
- Recommended standards for energy calibration:

  Helmer and Van der Leun (Nucl. Instr. and Meth. in Phys. Res. **A450**, 35 (2000)
- Not observed, but expected (From level energy difference)
- Deduced from conversion electron energies (Give atomic electron binding energy)
- Multiplets:

  Broader peak in spectrum
  Known levels involved

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Recommended standards for γ-ray energy calibration (1999)

R.G. Helmer[a,*], C. van der Leun[b,*]

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- Uncertainties: Statistical

Give (in comments) estimate of systematic errors.

When uncertainties are known to include systematic errors, no result from weighted average should have an uncertainty smaller than the smallest on the input uncertainty.

No uncertainty should be smaller than the uncertainty in the calibration standard.

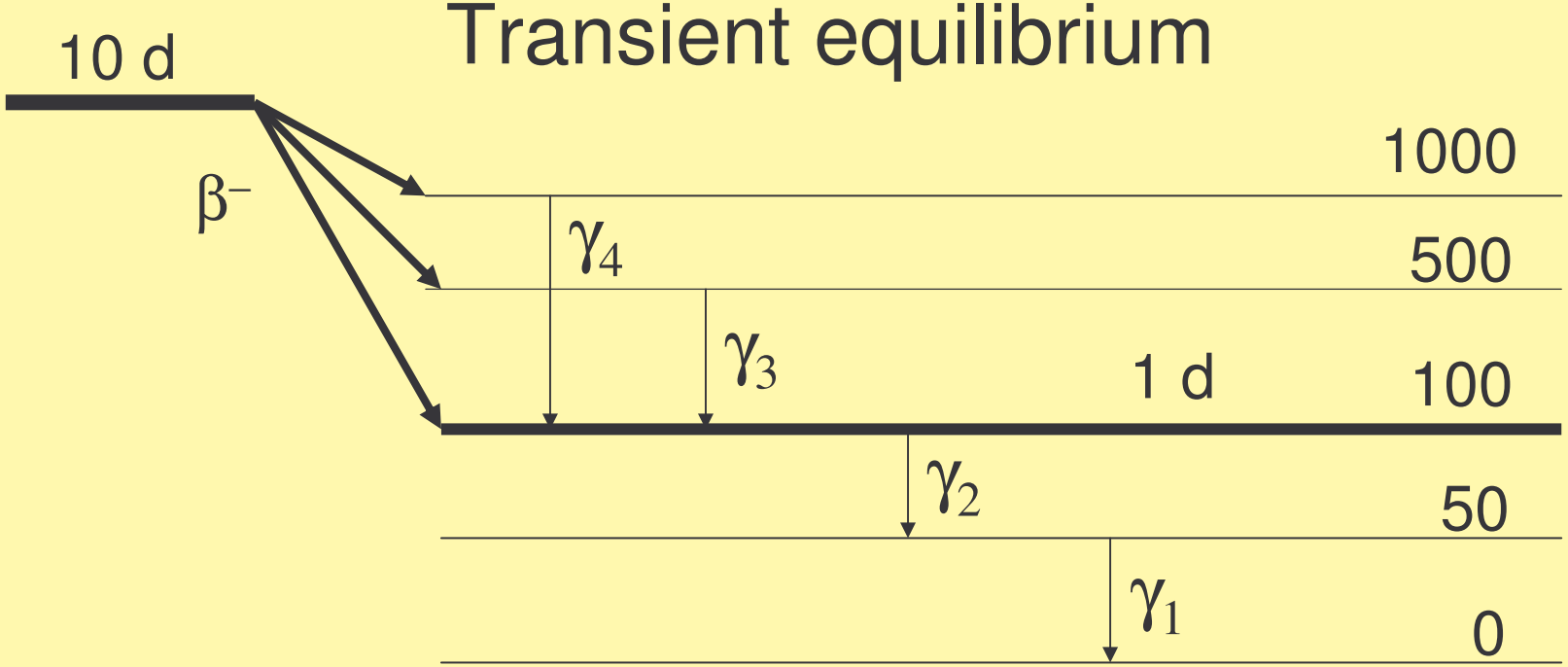
Uncertainties larger than *25* should be rounded off.

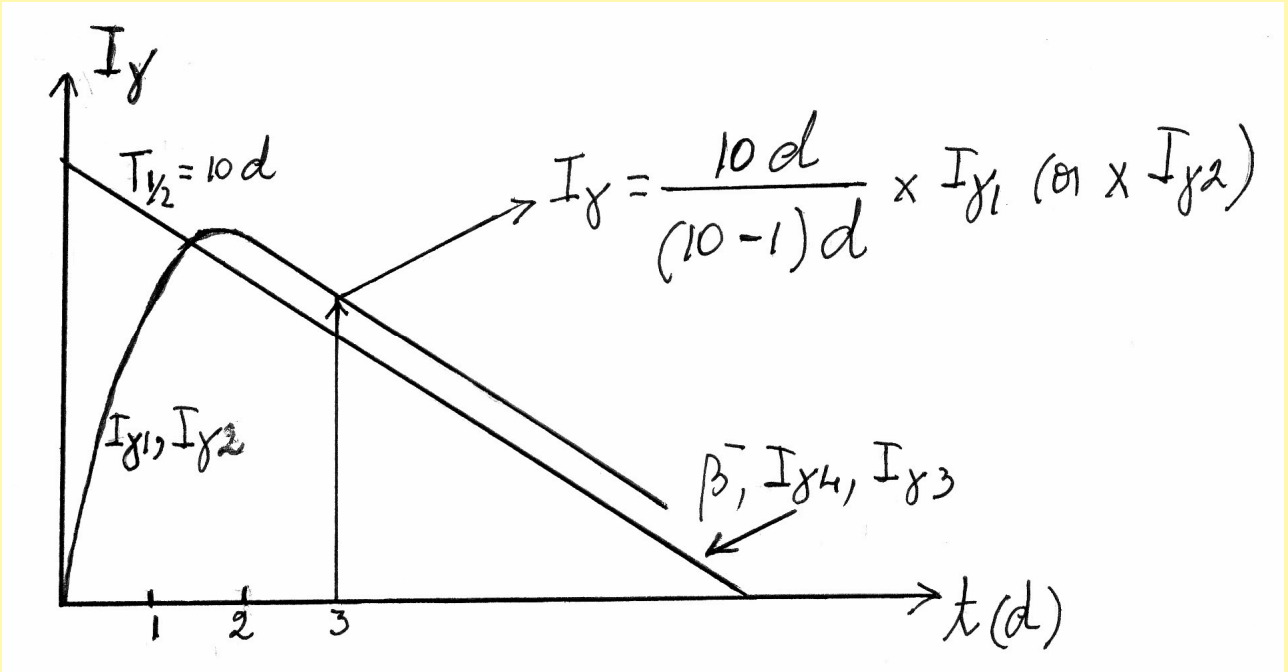
Author	ENSDF
351.53 ± 0.25	351.53 *25*
351.53 ± 0.30	351.5 *3*
8346 ± 29	83.5E2 *3*

2. Relative intensity

- Weighted average from radioactive decay
- Use 100 for the most intense gamma ray.
- Use a limit for an expected (but unobserved) γ ray.
- Use total transition intensity (TI) if this is the only quantity measured, or deduced from transition intensity balance. If α_T is known, then deduce and give I_γ.
- Limits are acceptable (e.g. $I_\gamma < A$), but $I_\gamma = ½\ A \pm ½\ A$ is preferable (for calculating transition intensity balances).
- Intensity from an isomer in the daughter nucleus should not be given if such intensity is time dependant. Include a comment giving the percent feeding to the isomer, and explain the reason for not giving I_γ.

Transient equilibrium





3. <u>Multipolarity and mixing ratio (δ)</u>

- From conversion electron data. If I_K and I_γ were used to determine α_K, explain normalization between electron and photon intensity scales. Conversion electron sub-shell ratios.
- From γ-ray angular correlations ($\gamma(\theta)$). Notice that $\gamma(\theta)$ determines *only* the L component of the γ-ray character, thus mult.= D, D+Q, etc. $T_{1/2}$(exp.) may be used to rule out choices. For example, Q=M2 and D+Q=E1+M2.

Multipolarity and mixing ratio (δ) from conversion electron data

- Using experimental conversion coefficients

δ^2= E2 γ-ray intensity / M1 γ-ray intensity = $I_\gamma(E2)/I_\gamma(M1)$ …. (1)

$$I_\gamma(M1) + I_\gamma(E2) = I_\gamma \text{ …. (2)}$$

From equations (1) and (2) we obtain:

$$I_\gamma(M1) = I_\gamma / 1 + \delta^2, \text{ and } I_\gamma(E2) = I_\gamma\, \delta^2 / 1 + \delta^2$$

Conversion electron intensity: $I_e = I_e(M1) + I_e(E2)$

Experimental conversion coefficient

$$\alpha(exp) = I_e/ I_\gamma = 1/ I_\gamma\, [I_\gamma(M1) \times \alpha(M1)^{th} + I_\gamma(E2) \times \alpha(E2)^{th}]$$

$$\text{or, } \alpha(exp) = 1/ I_\gamma\, [I_\gamma / 1 + \delta^2 \times \alpha(M1)^{th} + I_\gamma\, \delta^2 / 1 + \delta^2 \times \alpha(E2)^{th}]$$

$$\boxed{\delta^2 = (\alpha(M1)^{th} - \alpha(exp)) / (\alpha(exp) - \alpha(E2)^{th})}$$

$$\%M1 = 100/1 + \delta^2, \quad \%E2 = 100\, \delta^2 / 1 + \delta^2$$

- Using experimental electron sub-shell ratios

$$R(exp) = I_e(L1)/ I_e(L3)$$

Then

$$\delta^2 / 1 + \delta^2 = A / [\alpha(E2,L1)^{th} - \alpha(M1,L1)^{th} + R(exp)\ (\alpha(M1,L3)^{th} - \alpha(E2,L3)^{th})]$$

where

$$A = R(exp)\ \alpha(M1,L3)^{th} - \alpha(M1,L1)^{th}$$

- Consistency of entries for α and δ:

For a single multipolarity the δ field should be blank.

For $\delta < V$:

Give *only* dominant multipolarity and corresponding α. Give $\delta < V$ in a comment, or give both multipolarities and $\delta < V$ in the δ field. Calculate α from $\delta = ½\ V \pm ½\ V$.

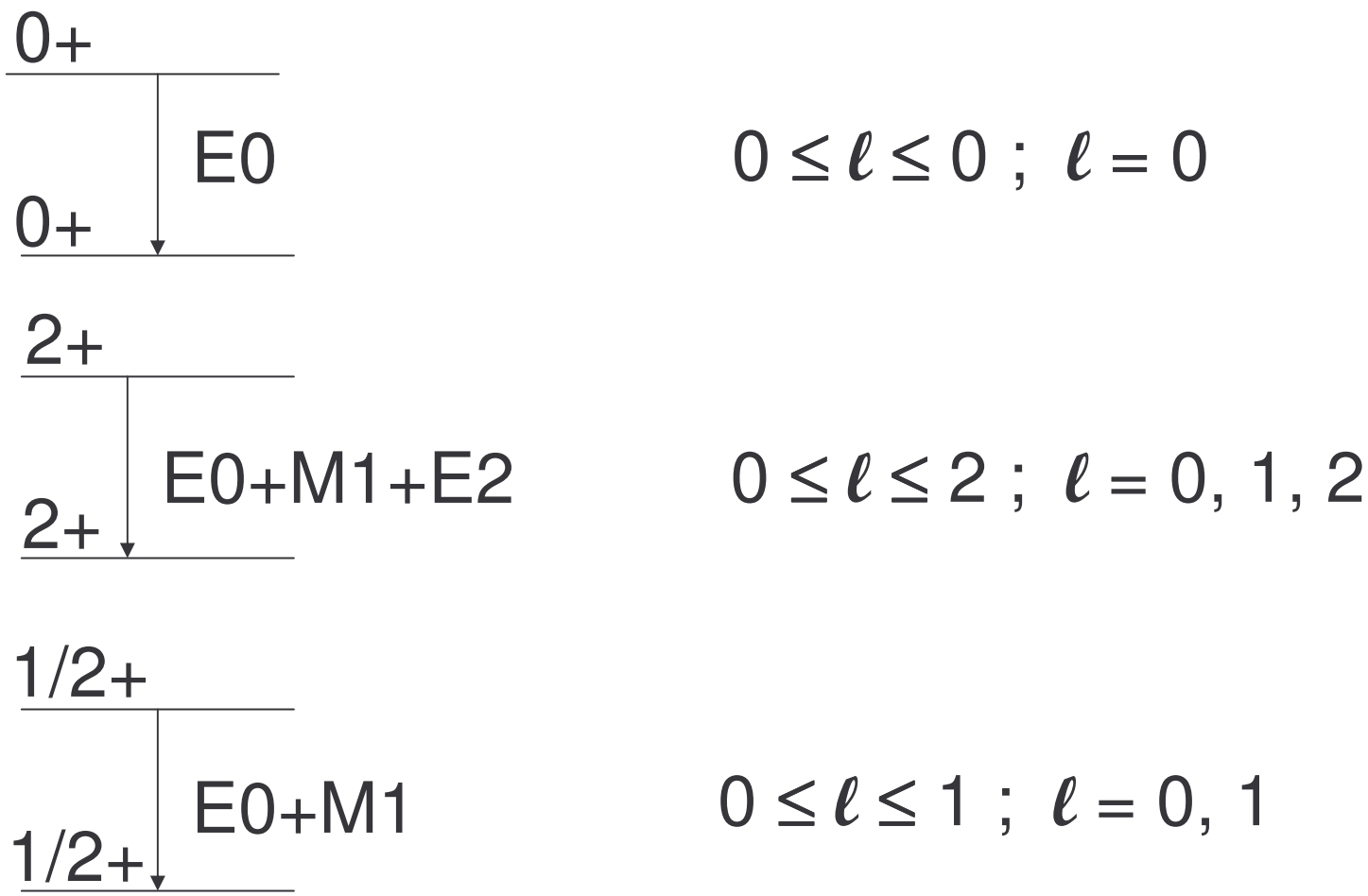
Examples: E2+M3 with $\delta < 0.5$ should preferably be entered as E2, whereas M1+E2 with $\delta < 0.5$, as M1+E2 ($\delta = 0.25 \pm 0.25$).

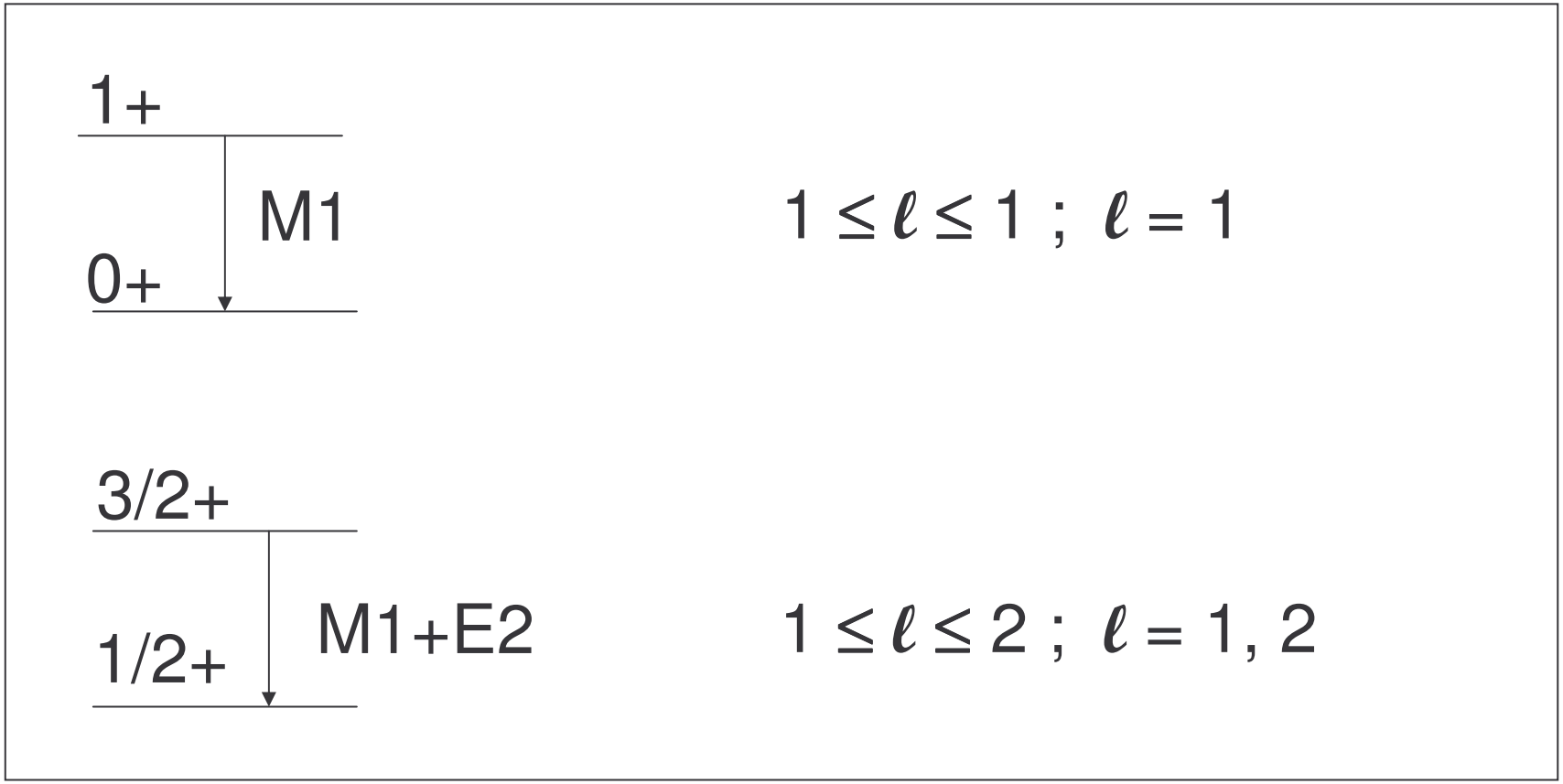
M1, E2 is not the same as M1+E2.

- Assumed multipolarity

[M1], [E2], [M1+E2], [M4], etc.

More about multipolarities




1+
M1
0+
$1 \leq \ell \leq 1 \; ; \; \ell = 1$
3/2+
M1+E2
1/2+
$1 \leq \ell \leq 2 \; ; \; \ell = 1, 2$

4. Internal conversion coefficients

- Theoretical values:

  From Hager and Seltzer (1968Ha53) for K, L_i, M_i shells, and $Z \geq 30$

  From Dragoun et al. (1971Dr11) for N, O, … shells.

  From Dragoun et al. (1971Dr09) for N_i shells.

  From Band et al. (1976Ba63) for $E_\gamma \leq 6000$ keV, Z=3, 6, 10, and $14 \leq Z \leq 30$.

  From Trusov (1972Tr09) for $E_\gamma > 2600$ keV.

  From Hager and Seltzer (1969Ha61), K/L_1, L_1/L_2, for E0 transitions.

New Calculation of Conversion Coefficients

Dirac-Fock Internal Conversion Coefficients

I.M. Band, M.B. Trzhaskovskaya, C.W. Nestor, Jr., P.O. Tikkanen, and S. Raman

Atomic Data and Nuclear Data Tables **81**, 1 (2002)

(To be discussed by Tom Burrows)

- Experimental values:

For very precise values ($\leq$ 3% uncertainty).

E_γ = 661 keV ; ^{137}Cs (α_K=0.0902 $\pm$ 0.0008, M4)

Nuclear penetration effects.

^{233}Pa β^- decay to ^{233}U.

E_γ = 312 keV almost pure M1 from electron sub-shell ratios.

However α_K(exp) = 0.64 $\pm$ 0.02.

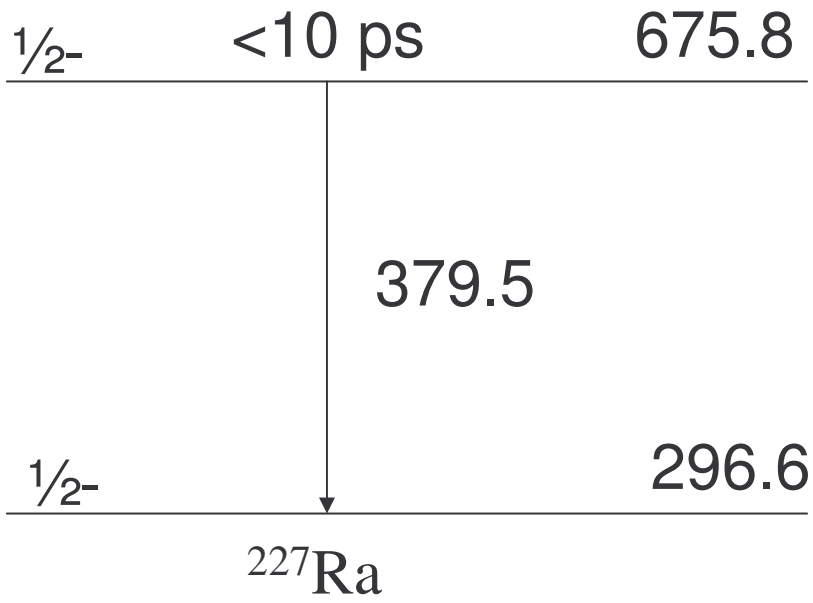
(α_K th(M1)=0.78, α_K th(E2)=0.07)

For mixed E0 transitions (e.g., M1+E0).

^{227}Fr β^- ^{227}Ra

E_γ = 379.1 keV (M1+E0); α(exp) = 2.4 $\pm$ 0.8

α^{th}(M1) = 0.40; α^{th}(E2) = 0.08



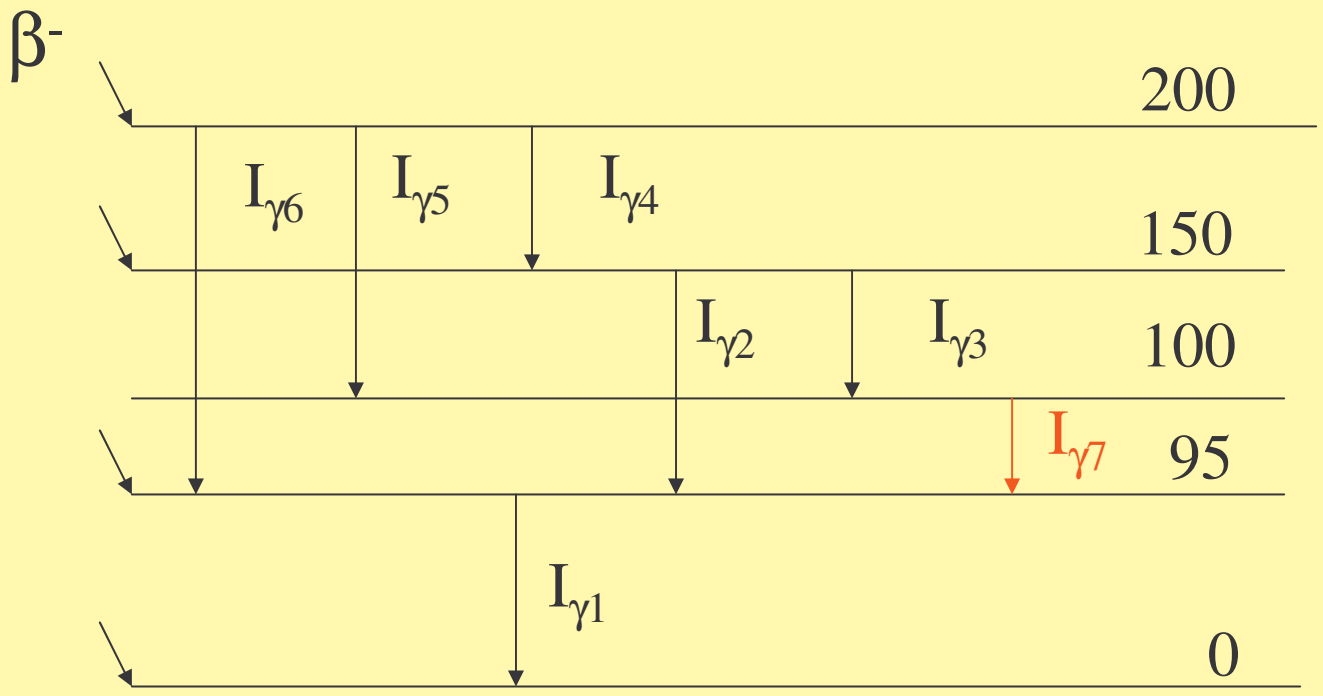
- Total transition intensity

The TI field should be used *only* if TI (rather than I_γ) is the measured or deduced quantity. Usual cases are:

TI deduced from transition intensity balance.

TI = Σ I_i(ce), if I_γ is known to be negligible. If not, but conversion coefficient is known, then deduced and give I_γ.

Total intensity from transition-intensity balance



$TI(\gamma_7) = TI(\gamma_5) + TI(\gamma_3)$

If $\alpha(\gamma_7)$ is known, then

$I\gamma_7 = TI(\gamma_7) / [1 + \alpha(\gamma_7)]$

5. Absolute intensities

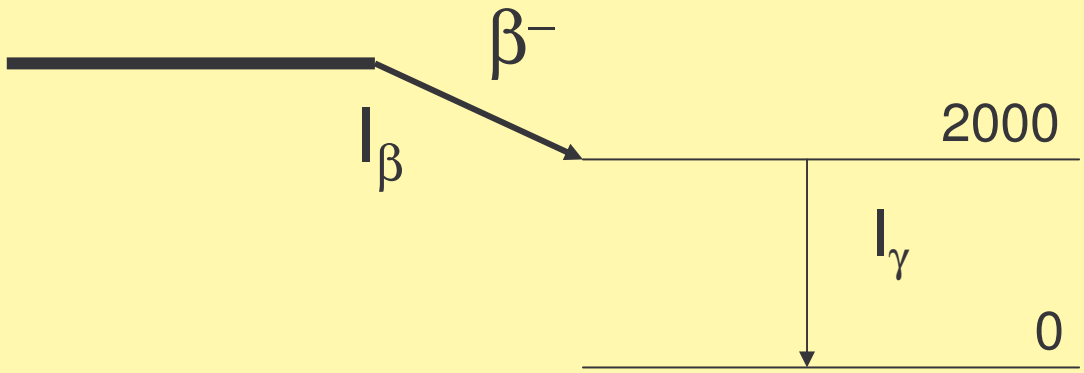
   “Intensities per 100 disintegrations of the parent nucleus”

- Measured (Photons from β^-, $\varepsilon+\beta^+$, and α decay)

  Simultaneous singles measurements

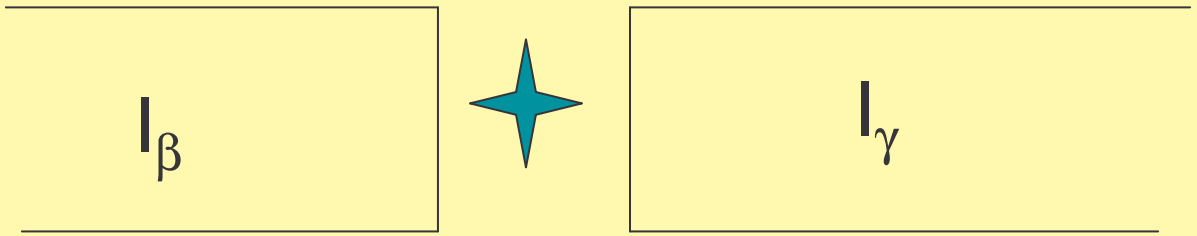
  Coincidence measurements

Absolute γ-ray intensity



$$\gamma(\%) = I_\gamma / I_\beta = 100\%$$

Simultaneous singles measurement



I_β: β^- intensity corrected for detector efficiency

I_γ: γ-ray intensity corrected for detector efficiency

I_γ / I_β = absolute γ-ray intensity

Units: photons per β^- (or per 100 β^-) disintegrations

4. Decay scheme normalization

Rel. int.	Norm. factor	Abs. Int.
I_γ	NR × BR	$\%I_\gamma$
I_T	NT × BR	$\%I_T$
I_β	NB × BR	$\%I_\beta$
I_ε	NB × BR	$\%I_\varepsilon$
I_α	NB × BR	$\%I_\alpha$

BR: Factor for converting intensity per 100 *decays through this decay branch*, to intensity per 100 *decays of the parent nucleus*

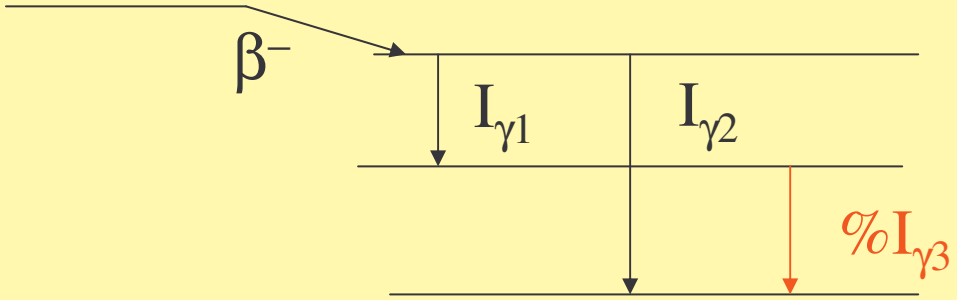
NR: Factor for converting relative I_γ to I_γ per 100 decays through this decay branch.

NT: Factor for converting relative TI to TI per 100 decays through this decay branch.

NB: Factor for converting relative β^- and ε intensities to intensities per *100 decays of this decay branch*.

Normalization Procedures

1. <u>Absolute intensity of one gamma ray is known</u> ($\%I_\gamma$)



Relative intensity $I_\gamma \pm \Delta I_\gamma$

Absolute intensity $\%I_\gamma \pm \Delta\%I_\gamma$

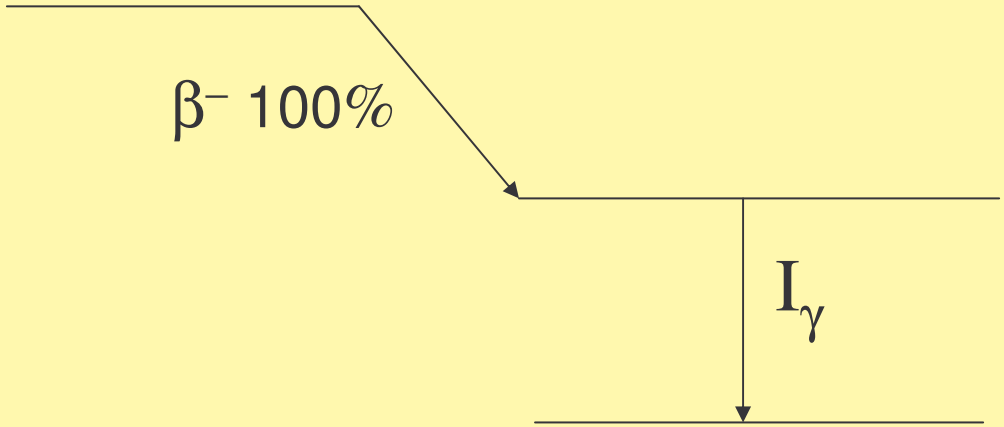
Normalization factor $N = \%I_\gamma / I_\gamma$

Uncertainty $\Delta N = [(\Delta\%I_\gamma / \%I_\gamma)^2 + (\Delta I_\gamma / I_\gamma)^2]^{1/2} \times N$

Then $\%I_{\gamma 1} = N \times I_{\gamma 1}$

$\Delta\%I_{\gamma 1} = [(\Delta N/N)^2 + +(\Delta I_\gamma / I_\gamma)^2]^{1/2} \times I_{\gamma 1}$

2. From Decay Scheme



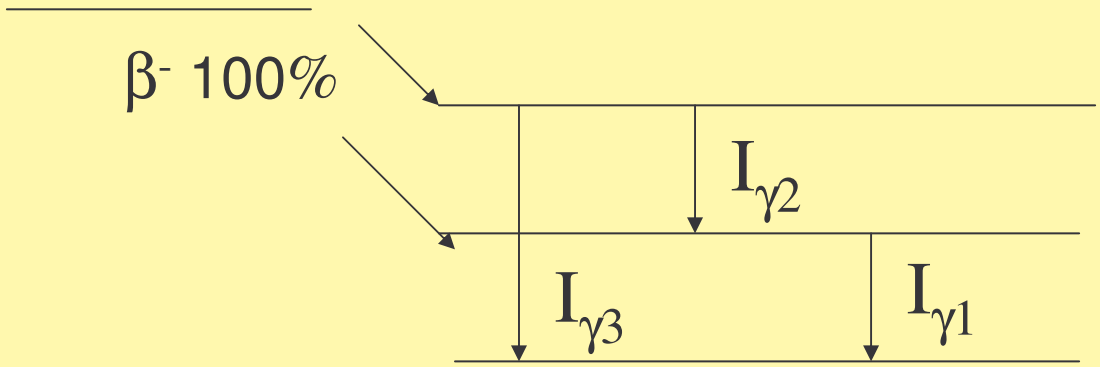
Iγ: Relative γ-ray intensity; α: total conversion coefficient

$$N \times I_\gamma \times (1 + \alpha) = 100\%$$

Normalization factor $N = 100/ I_\gamma \times (1 + \alpha)$

Absolute γ-ray intensity $\% I_\gamma = N \times I_\gamma = 100/ (1 + \alpha)$

Uncertainty $\Delta\% I_\gamma = 100 \times \Delta\alpha/(1 + \alpha)^2$



Normalization factor $N = 100 / I_{\gamma 1}(1 + \alpha_1) + I_{\gamma 3}(1 + \alpha_3)$

$\% I_{\gamma 1} = N \times I_{\gamma 1} = 100 \times I_{\gamma 1} / I_{\gamma 1}(1 + \alpha_1) + I_{\gamma 3}(1 + \alpha_3)$

$\% I_{\gamma 3} = N \times I_{\gamma 3} = 100 \times I_{\gamma 3} / I_{\gamma 1}(1 + \alpha_1) + I_{\gamma 3}(1 + \alpha_3)$

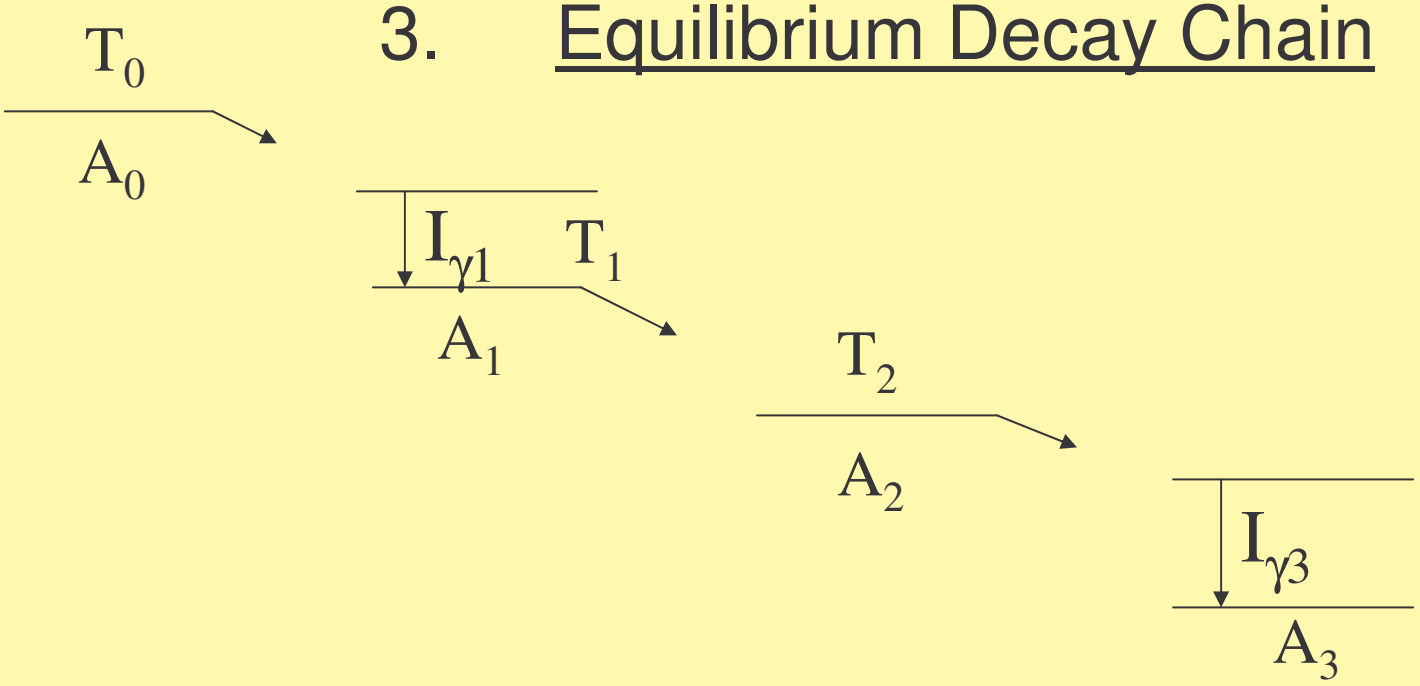
$\% I_{\gamma 2} = N \times I_{\gamma 2} = 100 \times I_{\gamma 2} / I_{\gamma 1}(1 + \alpha_1) + I_{\gamma 3}(1 + \alpha_3)$

Calculate uncertainties in $I_{\gamma 1}$, $I_{\gamma 2}$, and $I_{\gamma 3}$. Use 3% fractional uncertainty in α_1 and α_3.

See Nucl. Instr. and Meth. **A249**, 461 (1986).

To save time use computer program GABS

3. Equilibrium Decay Chain



$T_0 > T_1, T_2$ are the radionuclide half-lives,

For $t = 0$ only radionuclide A_0 exists,

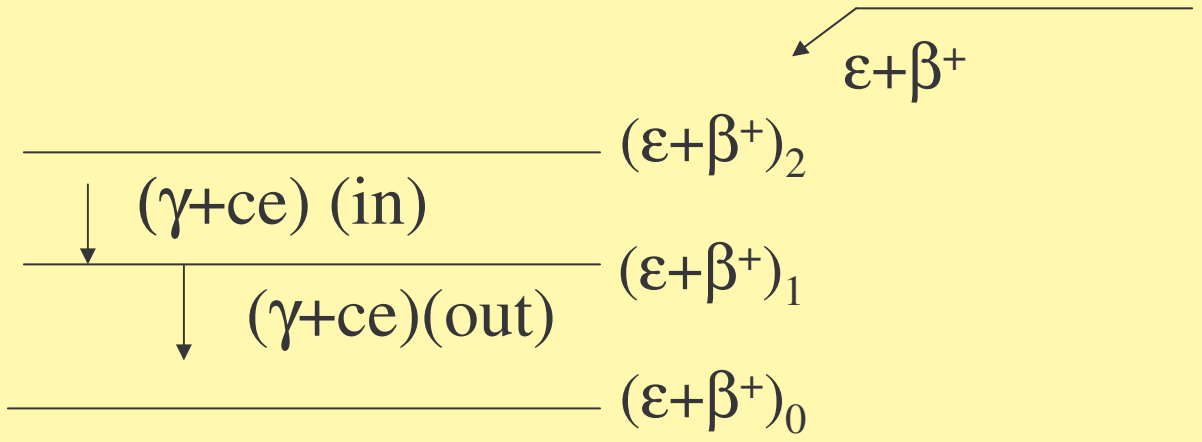
$\%\ I_{\gamma 3}$, $I_{\gamma 3}$, and $I_{\gamma 1}$ are known.

Then, at equilibrium

$$\%\ I_{\gamma 1} = (\%\ I_{\gamma 3}/I_{\gamma 3}) \times I_{\gamma 1} \times (T_0/(T_0 - T_1) \times (T_0/(T_0 - T_2)$$

Normalization factor $N = \%I_{\gamma 1}/ I_{\gamma 1}$

4. Annihilation radiation intensity is known



$I(\gamma\pm)$ = Relative annihilation radiation intensity

X_i = Intensity imbalance at the ith level = (γ+ce) (out) – (γ+ce) (in)

$r_i = \varepsilon_i / \beta^+_i$ theoretical ratio to ith level

$X_i = \varepsilon_i + \beta^+_i = \beta^+_i \ (1 + r_i)$, therefore $\beta^+_i = X_i / 1 + r_i$

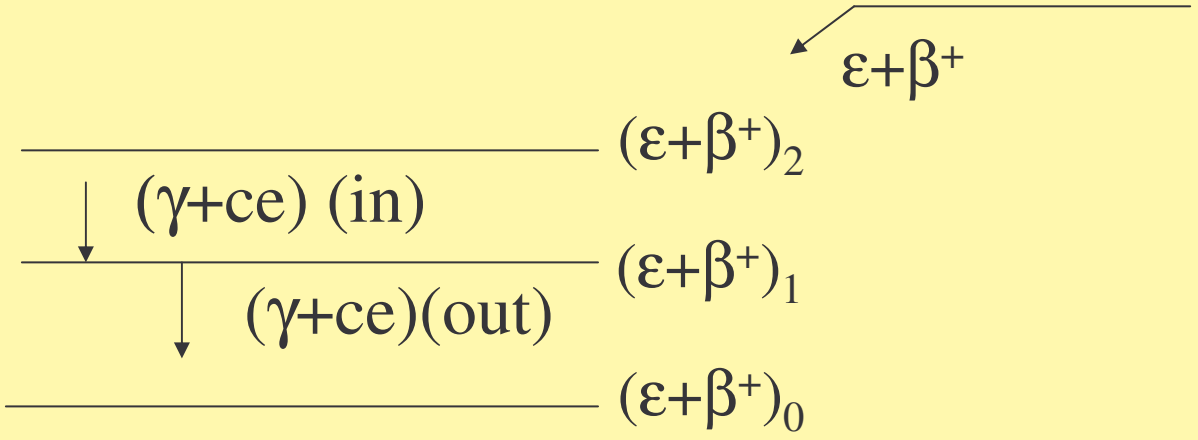
$$2 \left[X_0 / (1 + r_0) + \Sigma\, X_i / (1 + r_i)\right] = I(\gamma\pm) \ \ldots\ldots\ldots (1)$$

$$\left[X_0 + \Sigma\, I_{\gamma i}\ (\gamma + ce) \text{ to gs } \right] N = 100 \ \ldots\ldots\ldots\ (2)$$

Solve equation (1) for X_0 (rel. gs feeding).

Solve equation (2) for N (normalization factor).

5. X-ray intensity is known



I_K = Relative Kx-ray intensity

X_i = Intensity imbalance at the ith level = (γ+ce) (out) – (γ+ce) (in)

$r_i = \varepsilon_i / \beta^+_i$ theoretical ratio to ith level

$X_i = \varepsilon_i + \beta^+_i$, so $\varepsilon_i = X_i r_i / 1 + r_i$ (atomic vacancies); ω_K=K-fluorsc.yield

P_{Ki} = Fraction of the electron-capture decay from the K shell

$$I_K = \omega_K [\varepsilon_0 \times P_{K0} + \Sigma \varepsilon_i \times P_{Ki}]$$

$$I_K = \omega_K [P_{K0} \times X_0 r_0 / (1 + r_0) + \Sigma P_{Ki} \times X_i r_i / 1 + r_i] \ldots (1)$$

$$[X_0 + \Sigma I_i(\gamma + ce) \text{ to gs}] N = 100 \ldots . (2)$$

Solve equation (1) for X_0, equation (2) for N.

5. Beta particles

1. Energy (keV)

- Give E_β(max) *only* if experimental value is so accurate that it could be used as input to mass adjustment.
- Do not give E_β(avg.), program LOGFT calculates its value.

2. Absolute intensity (%I_β, per 100 decays of the parent nucleus)

- Give experimental value, if used for normalizing the decay scheme.
- Give absolute value deduced from γ-ray transition intensity balance (Program GTOL).

3. Log*ft*

   Usually authors assign spins and parities. Nevertheless, verify that the relevant log*ft* values are consistent with their assignments.

6. Electron capture

- Give ($I_\varepsilon + I_{\beta+}$) feedings deduced from γ-ray transition intensity balance. Program LOGFT calculates (from theory) ε and β^+ probabilities.
- Program LOGFT calculates (from theory) sub-shell (P_K, P_L, P_M, …) probabilities.
- Give (in comments) x-ray intensities. These are useful for normalizing or testing the decay scheme.

7. Alpha particles

- Energy (keV)

Most measurements are relative to a line from a standard radionuclide. Include this information in a comment.

Use Ritz's (At. Data and Nucl. Data Tables **47**, 205 (1991)) evaluated E_α and I_α when no new values are available.

- Intensity

Give intensities preferably "per 100 α decays" (NB=1), and a branching factor BR to convert them to "per 100 decays of the parent nucleus.

- Hindrance factor

HF= experimental $T_{1/2}(\alpha)$/theoretical $T_{1/2}(\alpha)$. The theoretical value is from 1947Pr17 (M.A. Preston). The assumption is that 0^+ to 0^+ α transitions from even-even nuclei are the fastest (HF=1). These transitions are used to determine the radius parameter r_0 (See 1998Ak04, Y.A. Akovali). Use program ALPHAD.

Favored alpha-particle transition

- HF < 4
- Takes place between levels with the same spin and parity

The radius parameter r_0 (Y. Akovali, Oak Ridge)

- Odd-N nucleus (Z, A)

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

- Odd-Z nucleus (Z, A)

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

- Odd-Odd nucleus (Z, A)

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

  $[r_0(Z-1, N+1)+r_0(Z-1, N-1)+r_0(Z+1, N+1) +r_0(Z+1, N-1)]/4$

Example

$^{219}Rn \Rightarrow ^{215}Po$ (Odd-N)

r_0 (Z=84, N=131) = [r_0(84, 130) + r_0(84, 132)] /2

From 1998Ak04:

r_0(84,214) = 1.559 *8*

r_0(84,216) = 1.5555 *2,* therefore

r_0 (Z=84, N=131) = 1.557

Use Table 1 – "Calculated r_0 for even-even nuclei" (1998Ak04). Insert R0= … in *comment* record:

CA HF R0=…

Run program ALPHAD to calculate hindrance factors.

8. Level structure and decay scheme