

# GOSIA calculations [exercises]

gosia < sample.inp

Manual: [www.slcyj.uw.edu.pl/gosia](http://www.slcyj.uw.edu.pl/gosia)

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# Before you start

- Do the **research**: what do you know about the isotope of interest: go through the data base, check the **level scheme**, look for known **lifetimes**, **branching ratios**,  $B(E0, E1, E2, E3..)$ ,  $B(M1)$ , **mixing ratios**, **quadrupole moments**. If you are lucky and you find some spectroscopic data for your nucleus, recalculate the transition strengths into matrix elements. **Read the papers. If something is evaluated in the data basis as an average value it doesn't mean it is the value you should use!**
- **Ask theorists!**
- <http://bricc.anu.edu.au/> - **electron conversion coefficient** calculator
- Calculate the **SAFE energy**
- What is the **beam**? Be sure about the energy and scattering angles
- What is the **target**? How thick? How complex? Energy loss of the beam in the target material is important (ELO, SRIM programs)
- **Normalization** method: known target excitation or lifetimes?
- **Detectors**:
  - **Gamma array**: how many? How far from the target? Material? Size? Efficiency?
  - **Particle array**: theta and phi angles, the geometry (CD, PIN, MCP...), dead pixels, useful detection range?

# GOSIA input structure

1. OP,FILE – header files (TAPES)
2. OP,TITL
3. OP,GOSI (with fit) - OP,COUL (without fit)
- LEVE
- ME
- EXPT
- CONT
- END,
4. OP,YIEL
5. OP,RAW
6. OP,INTG/INTI
7. OP,MINI
8. OP,ERRO
9. OP,POIN
10. OP,STAR
11. OP,THEO
12. OP, MAP
13. OP, REST
14. OP,GDET
15. OP,SIXJ

# GOSIA input file: **OP,FILE**

22 3 1

mini.out



Output file name

9 3 1

gdet.f9



OP,GDET output

8 3 1

gdet.f8



OP,GDET (if OP,RAW used)

12 3 1

matrix.me



Matrix elements

3 3 1

yield.f3



Gamma yields

4 3 1

corr.f4



Corrected gamma yields (after OP,INTG / INTI)

7 3 1

map.f7



OP,MAP output

14 3 1

sixj.14



OP,SIXJ output (if this option used)

0 0 0

# GOSIA input file: **OP,GDET**

## OP,FILE

22 3 1

gdet.out

output name

9 3 1

gdet.f9

GDET output file – parameters needed to reproduce  $\gamma$  energy dependence of the gamma detector solid angle attenuation coeff.  $Q_k$

8 3 1

gdet.f8

GDET output file – absorption coeff. needed to reproduce the detector efficiency, created if NPD is **negative** – related to “raw” spectra defined in OP,RAW

0 0 0

End of OP,FILE

## OP,TITL

Gamma detectors

Title

## OP,GDET

-1

0 9.5 14.0 22

0 0 0 0 0 0

OP,GDET input options

## OP,EXIT

**OP,GDET**

-2

0 9.5 14.0 22 !det1

0 0 0 0 0 0

0 9.5 14.0 22 !det2

0 0 0 0 0 0

**OP,EXIT**

NPD – number of **physically different** gamma detectors in use for all experiments defined in EXPT

**“-” for OP,RAW**

The distance from the target [cm]

The thickness of the Al absorber

The length of a crystal [cm]

The radius of the active core

The radius of the inactive core

# GOSIA input file: OP,GOSI

## LEVE

1	1	0	0.0
2	1	2	1.525
3	1	4	2.752
.	.	.	.
.	.	.	.
.	.	.	.
0	0	0	0

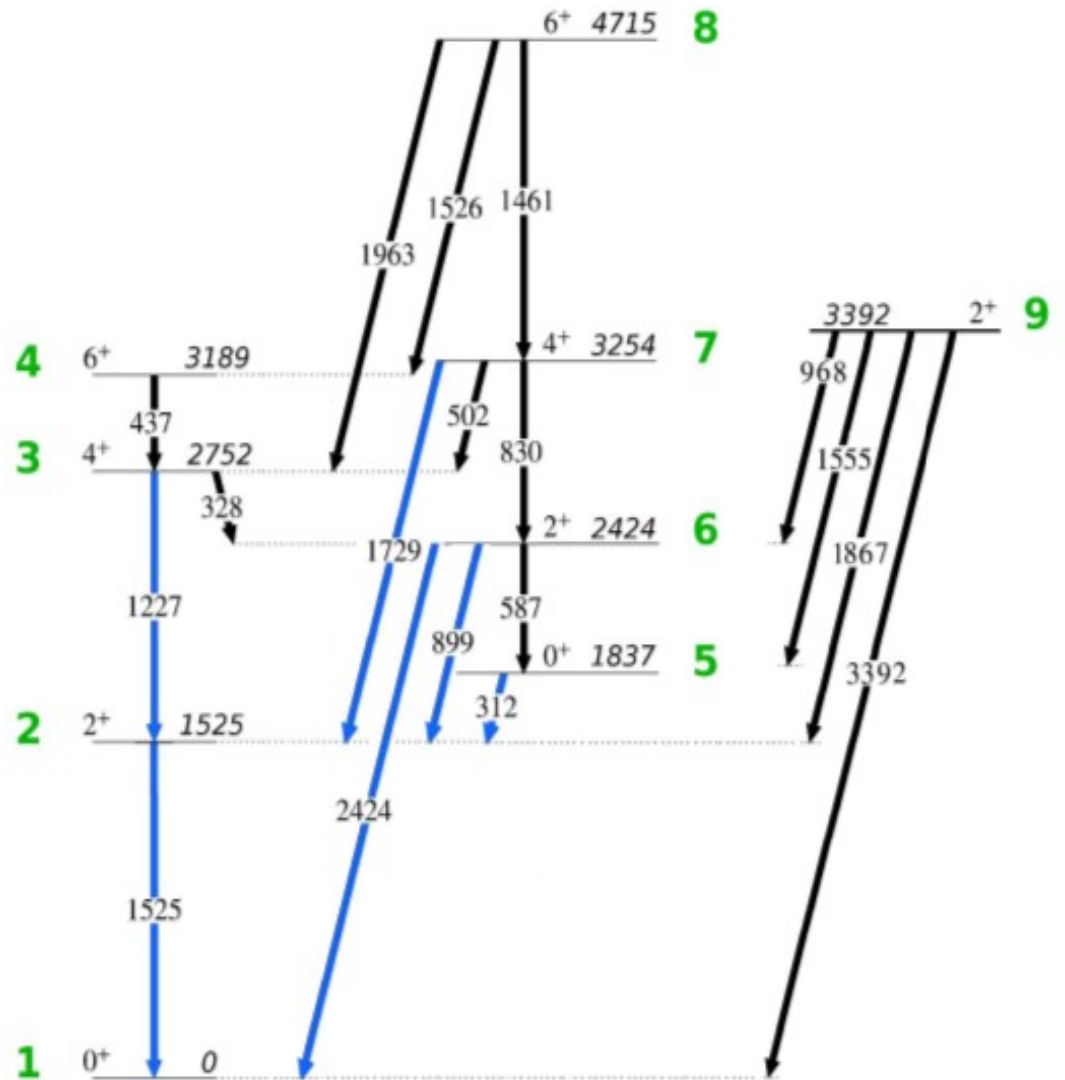
E [MeV]

SPIN

Parity

Level  
INDEX

1 = GROUND STATE



# GOSIA input file: **OP,GOSI**

```

ME
2 0 0 0 0
  1 2 0.20  0.0001  1.5
  2 6 0.08  -1.5    1.5
.
.
7 0 0 0 0
  2 6 1.01  -2.     2.
.
.
0 0 0 0 0

```

Multipolarity E(M) $\lambda$ :

1 E1

2 E2

3 E3

..

7 M1

8 M2

< INDEX1 || E(M) $\lambda$  || INDEX2 > [eb]

INDEX1 and INDEX2 are given in increasing order (start with INDEX1)

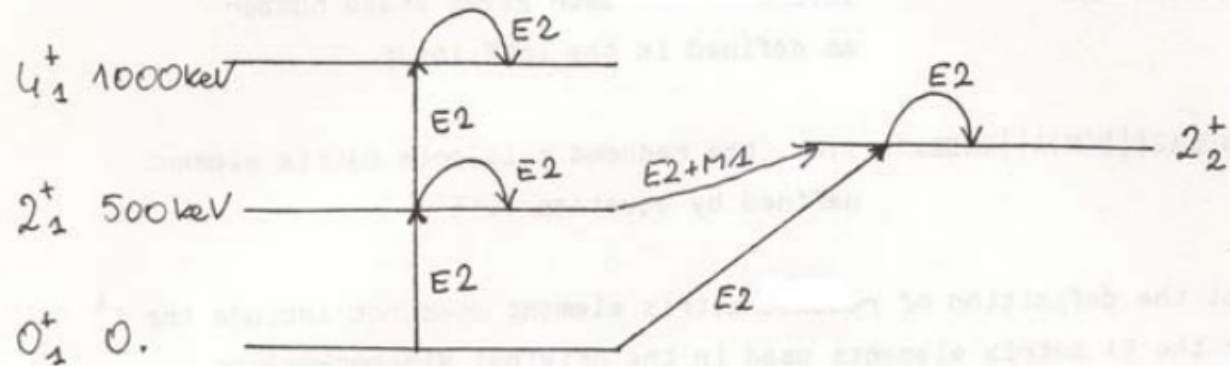
If "-" used before INDEX2  $\rightarrow$  COUPLING

**2 -6 0.08 1 2**

Limits for ME  
(R1 and R2)

INDEX1  
INDEX2

ME





# We need a set of ME to start with

## levels.inp

```
1 1 0 0.0
2 1 2 0.413
3 1 4 1.005
4 1 0 0.825
5 1 2 0.881
6 1 4 1.208
0 0 0 0
```

Level  
E[MeV]

SPIN

Parity

Level  
number

## megen levels.inp

```
1
Create setup for this multipolarity (y/n)
```

n

```
2
```

```
Create setup for this multipolarity (y/n)
```

y

```
Do you want them coupled ?
```

n

```
Please give limit value
```

```
-1.5 1.5
```

3

```
Create setup for this multipolarity (y/n)
```

n

```
(...)
```

```
7
```

```
Create setup for this multipolarity (y/n)
```

y

```
Do you want them coupled ?
```

n

```
Please give limit value
```

```
-1 1
```

8

```
Create setup for this multipolarity (y/n)
```

n

E2

M1

# We need a set of ME to start with

## levels.inp

```

1 1 0 0.0
2 1 2 0.413
3 1 4 1.005
4 1 0 0.825
5 1 2 0.881
6 1 4 1.208
0 0 0 0
    
```

Level  
E[MeV]

SPIN

Parity

Level  
number

## me.out

```

2 0 0 0 0
1 2 1 1.5 -1.5
1 5 1 1.5 -1.5
2 2 1 1.5 -1.5
2 3 1 1.5 -1.5
2 4 1 1.5 -1.5
2 5 1 1.5 -1.5
2 6 1 1.5 -1.5
3 3 1 1.5 -1.5
3 5 1 1.5 -1.5
    
```

E2

initial level	final level	starting value (1)	low limit	high limit
4	5	1	1.5	-1.5
5	5	1	1.5	-1.5
5	6	1	1.5	-1.5
6	6	1	1.5	-1.5

```

4 5 1 1.5 -1.5
5 5 1 1.5 -1.5
5 6 1 1.5 -1.5
6 6 1 1.5 -1.5
7 0 0 0 0
    
```

M1

```

2 2 1 1.0 -1.0
2 5 1 1.0 -1.0
3 3 1 1.0 -1.0
3 6 1 1.0 -1.0
5 5 1 1.0 -1.0
6 6 1 1.0 -1.0
0 0 0 0 0
    
```

# OP,THEO - COLLECTIVE MODEL ME

- generates the ME from rotational model
- generates only the matrix specified in the ME input and writes them to the output file
- For **in-band or equal-K** interband transitions only one intrinsic moment for a given multipolarity marked **Q1** is relevant.
- For **non-equal-K** values generally two moments with the projections equal to the **sum and difference of K's** are required (**Q1 and Q2**), (unless one of the K's is zero, when again only Q1 is needed)
- For the **K-forbidden** transitions a three parameter Mikhailov formula is used.

# OP,THEO - COLLECTIVE MODEL ME

## OP,THEO

2	Two bands
0,3	K of the gsb, # of levels
1,2,3	Level list for the gsb
2,3	K of the gamma band, # of levels
4,5,6	Level list for the gamma band
2	Multipolarity E2
1,1	In-band, gsb
1,0,0	Q1, two zeros irrelevant
1,2	Interband E2
1,1,0	Q1,Q2- Mikhailov formula, none of the K's=1/2, so Q3 irrelevant
2,2	In-band, gamma band
1,0,0	In-band Q1, Q2 and Q3 irrelevant
0,0	Ends E2 loop
7	M1 loop
1,2	Interband M1
1,1,0	Q1 and Q2 for Mikhailov formula
2,2	In-band M1
1,0,0	Q1 for in-band transitions
0,0	Ends M1 loop
0	Ends multipolarity loop and OP, THEO input

# OP,THEO for $^{188}\text{Hg}$ (EXAMPLE)

$$\langle KI_f \| \hat{M}(E2) \| KI_i \rangle = \sqrt{(2I_i + 1)} \langle I_i, K, 2, 0 | I_f K \rangle \sqrt{\frac{5}{16\pi}} eQ_0$$

OP,THEO

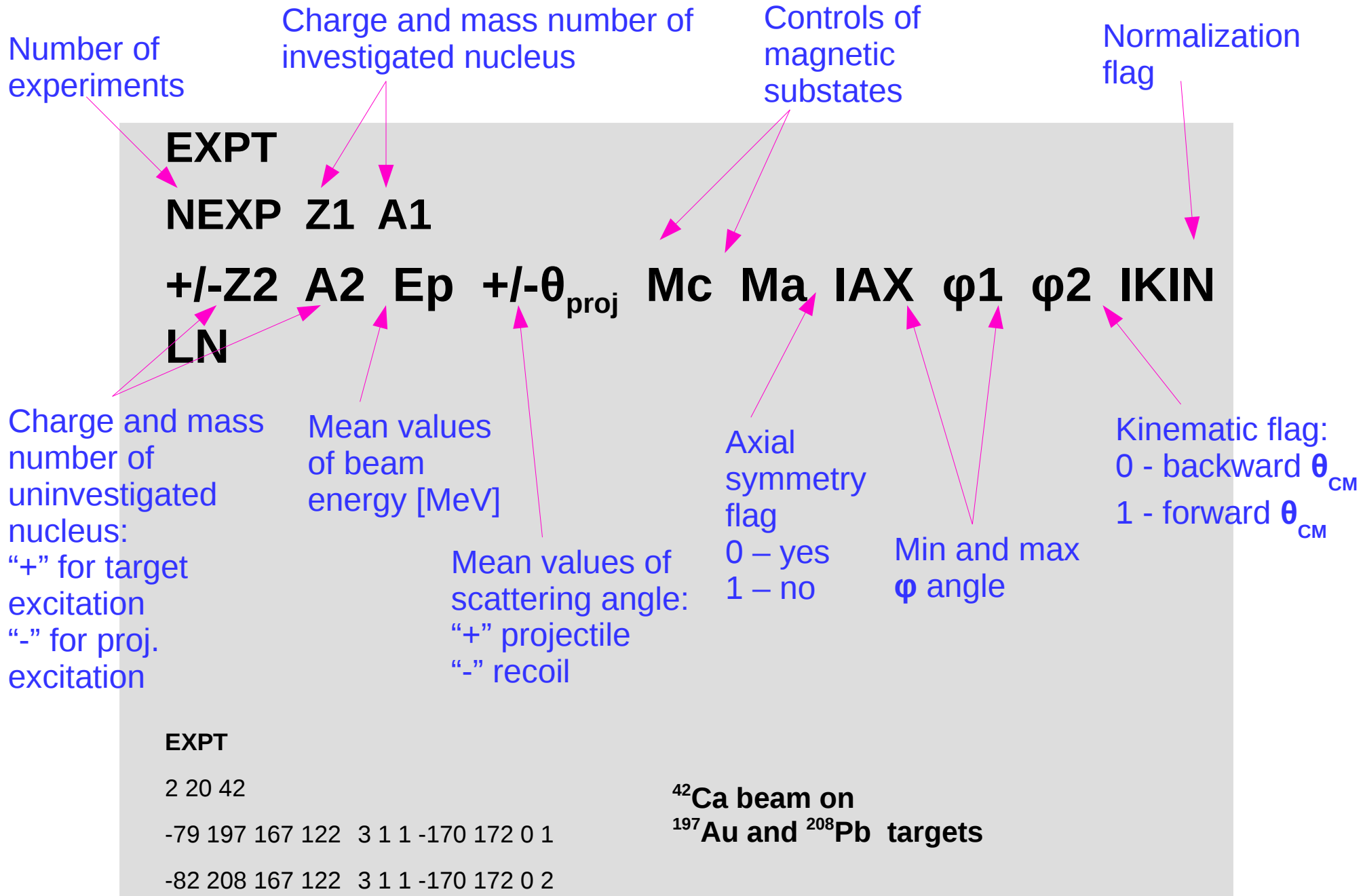
- 2 ← number of bands (2)
- 0,3 ← First band, K and number of states
- 1,2,3 ← band member indices
- 0,3 ← Second band, K and number of states
- 4,5,6 ← Multipolarity E2
- 2 ← Bands 1 and 1 (in-band)
- 1,1 ← Moment Q1 of the rotational band
- Q1,0,0
- 1,2
- Q1,0,0
- 2,2
- Q1,0,0
- 0,0 ← end of multipolarities loop
- 0 ← end of band-band input

*band 1*

*band 2*

$4^+$	<u>3</u>	1005		$4^+$	<u>6</u>	1208
$2^+$	<u>5</u>	881		$2^+$	<u>5</u>	881
$0^+$	<u>4</u>	825		$2^+$	<u>2</u>	413
$0^+$	<u>1</u>	0		$0^+$	<u>1</u>	0
$^{188}\text{Hg}$						

# GOSIA input file: **OP,GOSI: EXPT**



# GOSIA input file: OP,YIEL

OP,YIEL

0

**5 2**

0.1 0.3 0.5 1.0 1.5

**1**

0.000829 2.41E-5 5.60E-6 1.143E-6 0.000269

**2**

0.01175 0.0001328 2.06E-5 2.59E-6 8.94E-5 0.000314

**5 2**

1 2 3 4 5

25 55 85 130 172

40 75 270 325 59

1 2 3 4 5

25 55 85 130 172

40 75 270 325 59

**2 1**

1 !EXP1

0.001 0.001 0.001 0.001 0.001

1 1 1 1 1

1 !EXP2

0.001 0.001 0.001 0.001 0.001

1 1 1 1 1

**3**

# GOSIA input file: **OP,YIEL**

```

OP,YIEL
0
5 2
0.1 0.3 0.5 1.0 1.5
1
0.000829 2.41E-5 5.60E-6 1.143E-6 0.000269
2
0.01175 0.0001328 2.06E-5 2.59E-6 8.94E-5 0.000314
5 2
1 2 3 4 5
25 55 85 130 172
40 75 270 325 59
1 2 3 4 5
25 55 85 130 172
40 75 270 325 59
2 1
1 !EXP1
0.001 0.001 0.001 0.001 0.001
1 1 1 1 1
1 !EXP2
0.001 0.001 0.001 0.001 0.001
1 1 1 1 1
3

```

## Electron conversion coefficients (BRICC)

number of energies and multi-polarities

Energy points [MeV]

Mult. 1

Coeff. for each energy point

Mult. 2

Coeff. for each energy point

Total number of gamma detectors for each exp

Numbers of gamma det. in GDET, exp 1

$\Theta$ , exp 1

$\Phi$ , exp 1

Numbers of gamma det. in GDET, exp 2

$\Theta$ , exp 2

$\Phi$ , exp 2

## NORMALIZATION transition

Number of data sets for exp. 1

Upper limits for all gamma det in exp 1

Relative normalization factors for each det. In exp 1

**NTAP** (0 for OP,POIN, OP,STAR, 3 if OP,CORR after integration is used, 4 if OP,MINI and ERRO is used)



# GOSIA input file: **OP,YIEL**

```
2 1.0
4 5 4 2 0.007 0.003
5 1 5 2 0.34 0.02

2 1.0
2 1.19 0.04
3 4.45 0.10

1 1.0
6 2 -0.18 0.02

1 1.0
2 2 2 -0.25 0.051
```

Number and weight of known branching ratios:  
Transition 1 (I2, I1), Transition 2 (I2, I1), BR,  $\Delta$ BR

Number and weight of known mean lifetimes [ps]  
Level index,  $\tau$ ,  $\Delta\tau$

Number and weight of of known  $\delta$ (E2/M1) mixing  
Transition,  $\delta$ ,  $\Delta\delta$

Number and weight of of known matrix elements  
multipolarity, I1, I2, ME,  $\Delta$ ME

```
0 0
0 0 in case nothing is known
0 0 about the investigated nucleus
0 0
```

# YIELD definition

## POINT

- One energy (E)
  - One angle ( $\Theta$ )
- as defined in EXPT  
use **OP,POIN**



## INTEGRATED

- Energy range  
( $E_{\min}$ - $E_{\max}$ )
  - Angular range  
( $\Theta_{\min}, \varphi_{\min}$  -  $\Theta_{\max}, \varphi_{\max}$ )
- as defined in **OP,INTG / INTI**



**Matrix elements values, excitation probability**

# TAPE 3 / 4 (experimental yields)

**IEXP** – exp. number – the same order as in EXPT and Op, YIEL

**1 1 20 42 167 3 1.0**

5 2 88 10

3 2 500 20

2 1 11000 100

**NG** – number of data sets for exp. IEXP (NDST in OP, YIEL)

**ZP** – proj. charge number

**AP** – proj. mass number

**EP** – proj. bombarding energy [MeV]

**ND** – of  $\gamma$ -rays for the specific IEXP and data set

**WT** – Weight

**li** – initial level index

**lf** – final level index

**Y** –  $\gamma$ -ray yield

**$\Delta Y$**  – absolute error of  $\gamma$ -ray yield

1 1 20 42 167 3 1.0

5 2 88 10

3 2 500 20

2 1 11000 100

# GOSIA input file: **OP,POIN**

- **NTAP = 0** in **OP,YIEL**
- This option evaluates the point gamma yield in the laboratory frame for the  $I_i \rightarrow I_f$  transition for **one energy** and **one particle scattering angle** given in **EXPT**

$$Y^{Point}(I \rightarrow I_f) = \sin(\theta_p) \int_{\phi_p} \frac{d^2\sigma(I \rightarrow I_f)}{d\Omega_\gamma d\Omega_p} d\phi_p$$

- includes the **Rutherford cross section**, the  $\sin(\Theta)$  term, integration over the projectile  $\varphi$  scattering angle, the deorientation effect and gamma-detector attenuation coefficients (from OP,GDET)
- Calculates the yield for one system – defined as one  **$\theta$ -E** point
- We use OP,POIN after OP,YIEL

0 – simulation, but not in use  
1 – “real” calculations, we use this option

**OP,POIN**  
**YFL YLIM**  
**1 0**

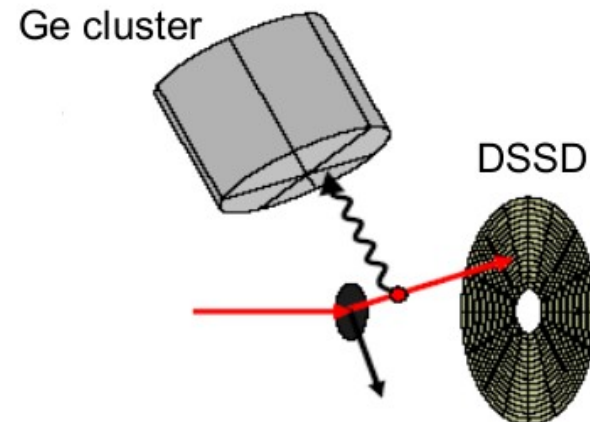
If **IFL=1** – if the transition specified in TAPE3 normalized to norm. transition in OP,YIEL exceed it, it is treated like the experimental observable and stored on TAPE4

- We use REAL detectors with continuous dimensions

# Why INTEGRATION?

- REAL conditions - GOSIA calculates **yields** from ME to get **realistic comparison** with experimental data
- integration over **solid angle** of the particle detectors, **energy loss in the target**, full correction for the velocity of the deexciting nucleus and the **deorientation effect** is included
- the Rutherford scattering is integrated over the particle detectors and energy loss in the target – an absolute normalization.
- the '**GOSIA yield**' may be understood as a mean differential cross section multiplied by a target thickness (in mg/cm<sup>2</sup>)

$$[Y] = [\text{mb/sr}] \times [\text{mg/cm}^2]$$



# GOSIA input file: **OP,INTG**

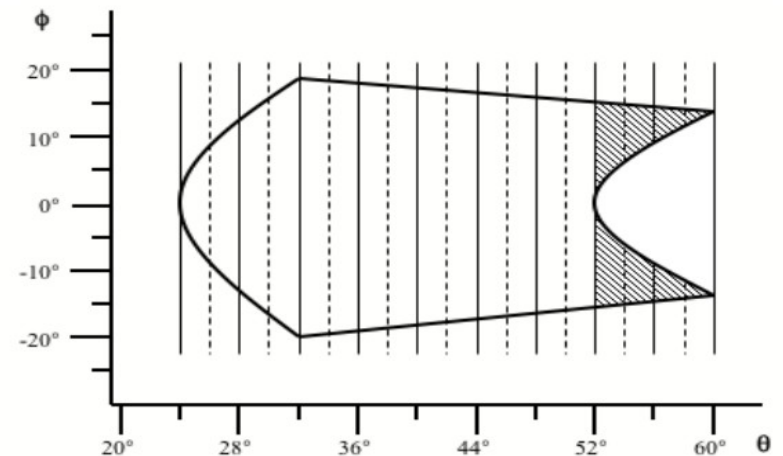
## 2 stages:

- $\gamma$  yields integrated over azimuthal angle  $\phi$  for each energy  $E$  and center-of-mass scattering angle  $\theta$  meshpoint (stored as an external array). The calculation of the meshpoint yields is repeated for each experiment (**as declared in EXPT**)
- integrate over bombarding energy  $E$  and the range of scattering angles  $\theta$  of the particle detectors which is performed by **interpolating** between the yields calculated at each  $E$ - $\theta$  meshpoint

(\*axial sym., circular detectors option recommended)

```
OP,INTG
NE +/-NT E_min E_max  $\theta$ _min  $\theta$ _max
E_1 E_2 ... E_NE
+/- $\theta$ _1 +/- $\theta$ _2 ... +/- $\theta$ _NE
NFI
 $\phi$ _1  $\phi$ _2 ...
NP
E_1 E_2 ... E_NP
(dE/dx)_1 (dE/dx)_2 ... (dE/dx)_NP
NI_1 NI_2
```

```
CONT
SPL,1. - SPILINES
END,
```



# GOSIA input file: OP,INTG

**OP,INTG**

**NE +/-NT  $E_{\min}$   $E_{\max}$   $\theta_{\min}$   $\theta_{\max}$**

Total number of E meshpoints,  $\theta$  meshpoints (“-” when the  $(\theta,\varphi)$  shape will be defined),  
Integration limits: minimum and maximum bombarding E [MeV] , minimum and maximum  
LAB angle of detected particle (in degrees)

**$E_1$   $E_2$  ...  $E_{NE}$**

Energy meshpoints (COULEX calculation performed for points)

**+/- $\theta_1$  +/- $\theta_2$  ... +/- $\theta_{NE}$**

Projectile scattering  $\theta$  meshpoints (COULEX calculation performed for points)

**NFI**

Number of  $\varphi$  ranges for  $\theta_i$  meshpoint - for  $\theta(\varphi)$  dependence (repeat for each  $\theta$ )

**$\varphi_1$   $\varphi_2$  ...**

NFI pairs of  $\varphi$  for  $\theta_i$  meshpoint (repeat for each  $\theta_i$ )

**NP**

Number of stopping power ( $3 < NP < 20$ ). If  $NP=0$ , values are taken from prev. exp.

**$E_1$   $E_2$  ...  $E_{NP}$**

Energy meshpoints in [MeV] for the stopping powers

**$(dE/dx)_1$   $(dE/dx)_2$  ...  $(dE/dx)_{NP}$**

Stopping powers in [MeV/(mg/cm<sup>2</sup>)]

**$NI_1$   $NI_2$**

Number of subdivisions in E ( $NI_1$ ) and projectile scatt. angle ( $NI_2$ ) used during the  
integration. EVEN and less than 100 both.

# GOSIA input file: OP,INTG - circular

Intensities for each Ge detector – circular particle detector  
option (with PIN diodes)

Calculate the  $\Delta\phi$  at each subdivision of  $\theta$  (**CONT CRD,#exp**)  
Circular det. approximation for PiN diodes (**CONT PIN,#PIN**)

**CONT**  
SMR,  
LCK,  
0,0  
INR,  
SPL,1.  
**CRD,1.**  
**1**  
**PIN,1.**  
**1,44**  
PRT,  
4,0  
2,0  
13,0  
14,0  
16,0  
5,1  
12,0  
18,1  
0,0  
END,

OP,INTG		$E_{\min}$	$E_{\max}$	$\theta$	$\phi$	$\theta_{1/2}$
NE	+/-NT					
$E_1$	$E_2 \dots E_{NE}$					



OP,INTG						
7	3	146.	152.	123.9	242.32	4.4 ! PIN6
146	147	148	149	150	151	152
7	3	146.	152.	123.9	298.28	4.4 ! PIN62
146	147	148	149	150	151	152
7	3	140.	152.	123.9	226.27	4.4 ! PIN68
146	147	148	149	150	151	152
7	3	140.	152.	123.9	98.32	4.4 ! PIN75
146	147	148	149	150	151	152
...						

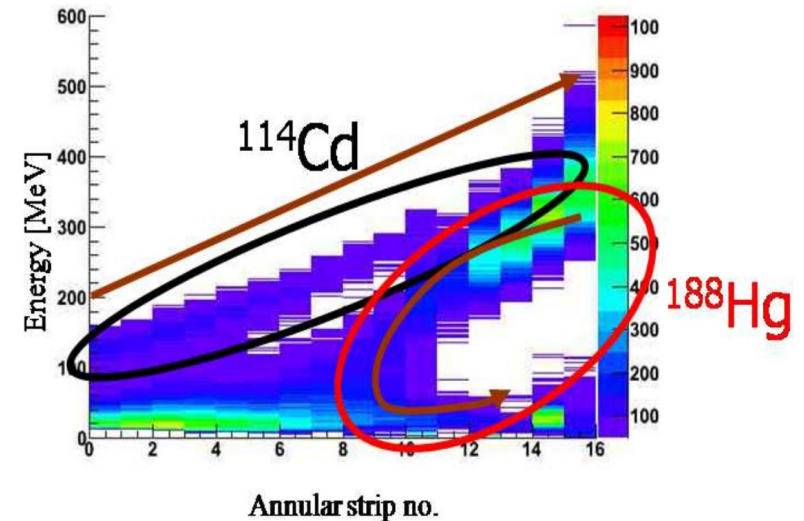


# GOSIA input file: OP,INTI

Developed to handle problems that occur for integration of systems involving inverse kinematics and when the **recoiling target nucleus is detected** (2 kinematic solution).

For each beam E and each angle the subroutine INVKIN calculates the appropriate value of kinematic flag and set it **automatically**

$\Theta$  angles always positive and correspond to laboratory scattering angles of the **detected particle**, that is, the angle of the scattered projectile if it is detected and the angle of the recoiling target nucleus if it is detected.



*N. Bree, PhD thesis, KULeuven,*

```
OP,INTI
NE +/-NT E_min E_max theta_min theta_max
E_1 E_2 ... E_NE
theta_1 theta_2 ... theta_NE
NFI
phi_1 phi_2 ...
NP
E_1 E_2 ... E_NP
(dE/dx)_1 (dE/dx)_2 ... (dE/dx)_NP
NI_1 NI_2
```

```
OP,INTI !for axial sym. and circ. det.
8 9 226 240 133 168
226 228 230 232 234 236 238 240
133 135 140 145 150 155 160 165 168
8
226 228 230 232 234 236 238 240
12.2 12.17 12.13 12.10 12.05 12.00 11.90 11.80
20,20
```

# YIELD correction

- Minimization of is usually performed using corrected yields
- Correction depends on the set of ME: GOSIA calculates the **point** yield ( $Y_p$ ) and the **integrated** yield ( $Y_I$ ) from the ME and gives the **correction factors CF** for each experimental yield (**OP,CORR** needed):

$$\mathbf{CF} = \frac{Y_P}{Y_I} \longrightarrow Y_{\text{exp}}^c = Y_{\text{exp}} \cdot \mathbf{CF}$$

After minimization the correction procedure should be repeated with a new set of ME (better fit, different correction) → until the solution is converged

- CF are calculated for **each** experimental yield

$^{42}\text{Ca}$  on  $^{197}\text{Au}$

$E_{\text{av}} = 167 \text{ MeV}$

$\Theta_{\text{av}} = 122^\circ$

EXPERIMENT 2			DETECTOR 1	
NI	NF	YEXP	YCOR	COR.F
3	2	.112E+00	.113E+00	.101E+01
6	1	.380E-01	.374E-01	.984E+00
6	2	.106E+00	.102E+00	.966E+00
5	2	.854E+00	.822E+00	.962E+00
2	1	.124E+02	.120E+02	.969E+00

# GOSIA AS A SIMULATION TOOL: YIELD $\Rightarrow$ COUNT RATE

$$Counts = 10^{-27} \cdot \left[ \frac{Q}{\hat{q}e} \right] \cdot \left[ \frac{N_A}{A} \right] \cdot [\rho dx] \cdot \text{Yintg} \cdot \Delta\theta_p \cdot \varepsilon_p \cdot \varepsilon_\gamma \cdot \Delta\Omega_\gamma$$

where:

$Q$  is the integrated beam charge [C]

$\hat{q}$  the average charges state of the beam

$e$  the proton charge [ $1.602 \times 10^{-19}C$ ]

$N_A$  Avogadro number [ $6.022 \times 10^{23}atoms/mol$ ]

$A$  Target mass number [g/mol]

$\rho dx$  areal target thickness in [a/cm<sup>2</sup>]

**Yintg from INTG or INTI** [ $\frac{mb}{sr \cdot rad}$ ]

$\Delta\theta_p$  Projectile scattering angle range [rad]

$\varepsilon_p$  particle detection efficiency per unit solid angle

$\varepsilon_\gamma$   $\gamma$ -ray detector efficiency excluding the geometrical solid angle

$\Delta\Omega_\gamma$  geometrical solid angle of the  $\gamma$ -ray detector. Note that usually one only knows the product  $\varepsilon_\gamma \cdot \Delta\Omega_\gamma$

$$\text{Count Rate} = \frac{7.6 \times 10^{-6} \times \text{yield} \times \text{current} [pps] \times \text{eff}}{A_{\text{target}}}$$

# GOSIA input file: **OP,RAW**

- This option needs energy-dependent efficiency calibration for each individual gamma detector (GREMLIN, EFFIT..)
- the first entry of **OP,GDET** should be negative to produce the **TAPE8**
- Need to declare which efficiency parametrization you need! (in **CONT**, flag **EFF**):  
0-Gremlin, 1-Jaeri, 2-Fiteff, 3-Leuven, 4-Radware
- **Do not use if all gamma intensities are efficiency-corrected**

```
CONT  
EFF,5  
1,0  
2,0  
3,0  
4,-1  
5,0  
END,
```

```
OP,RAW
```

```
IEXP
```

```
A1 A2 A3 A4 A5 A6 A7 A8
```

```
A1 A2 A3 A4 A5 A6 A7 A8
```

```
...
```

```
...
```

```
A1 A2 A3 A4 A5 A6 A7 A8
```

```
NC
```

```
ID1
```

```
I1 I2 ... I(ID1)
```

```
ID2
```

```
I1 I2 ... I(ID2)
```

```
...
```

```
...
```

```
0
```

number of the experiment (according to the sequence in **EXPT**)

gamma det. Eff. Parametrization, det 1 (as in **OP,GDET**)

gamma det. Eff. Parametrization, det 2

number of **CLUSERS**

number of Ge detectors in cluster 1

index numbers of Ge detectors in the cluster

number of Ge detectors in cluster 2

index numbers of Ge detectors in the cluster

End of the input

# GOSIA input file: **OP,MINI**

## $\chi^2$ function minimization

$$\chi^2 = \frac{1}{p} \left\{ \sum_{i=1}^{N \text{ exp}} \sum_{j=1}^{N \text{ det}} \sum_{k=1}^{N \gamma} \left[ \left( \frac{C_{ij} Y_k^{(T)} - Y_k^{(E)}}{\Delta Y_k^{(E)}} \right)^2 \right] \right. \\ \left. + \sum_{i=1}^{N s.d.} \left( \frac{d_i^{(T)} - d_i^{(E)}}{\Delta d_i^{(E)}} \right)^2 \right\}$$

normalisation factor

calculated yield

experimental yield

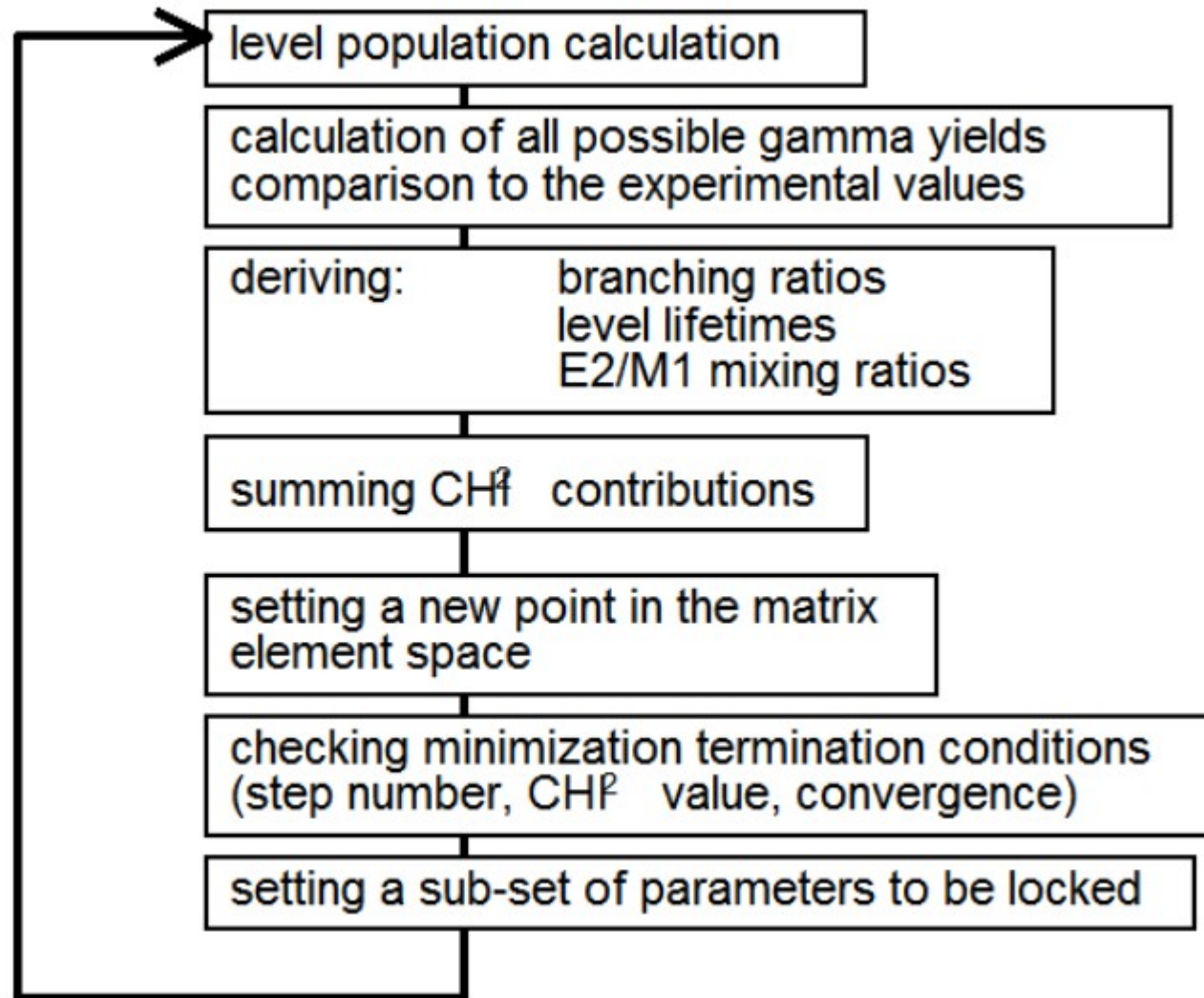
spectroscopic data point

calculated magnitude

The fitting procedure is continued, until the convergence of the  $\chi^2$  is achieved and the set of matrix elements optimally reproduce the experimental data.

Remember to run **OP,MAP** before **OP,MINI**, each time you change something in ME (insert OP,MAP command directly after OP,YIEL). This option stores the **q-parameters** important for **reorientation effect** (effective strength, related to the magnetic substates coupling) on **TAPE7**

# GOSIA input file: **OP,MINI**



# GOSIA input file: **OP,MINI**

## IMODE (4 digits):

1-fast approximation, 2-full COULEX formalism

0-simple steepest descent mini, 1-gradient mini with gradient derivative mode

0-absolute changes in values of ME will be used to improve the fit, 1-LOG values of ME used

0- absolute values of spectroscopic data will be used, 1-LOG values of spectroscopic data

1 – fixes all ME with absolute value of partial derivative is less than DLOCKS

**OP,MINI**

**IMODE IPTL CHILIM CONV TEST LOCKF NLOCK IFBL LOCKS DLOCKS**

The limit for LOCKS

max number of mini steps

convergence criterion  
 $|\overline{ME}_{n+1} - \overline{ME}_n| < CONV$

Stop criterion

TEST ≤ 1 – recalculation of the internal correction coeff. between fast approx. and full mini.

0 – forward difference method,  
 1 – forward-backward method

Number of ME to be locked if LOCKF=1 and CONV fulfilled

0 – mini will be terminated if CONV is fulfilled  
 1 – fix the NLOCK number of ME with the most significant derivative

```
OP,MINI
2100 20 0.0001 0.0001 1 1 1 1 1 0.0001
OP,EXIT
```

# GOSIA input file: **OP,ERRO**

- for estimating the error bars to be assigned to the set of matrix elements corresponding to the minimum value of  $\chi^2$  (**CONT CRF**), NTAP=4 (OP,YIEL)

0 – all ME (excluding fixed ones)

-1 – for ranges of ME (introduced later on)

0 – correlation matrix used

1 – correlation matrix not used

Mode flag:  
0 – diagonal  
1 – correlated

**OP,ERRO**  
**IDF MS MEND IREP IFC RMAX**

The largest floating point number available on a given computer

Repetition flag

0 – a new calculation (always for diag. Err.)

1 – read from TAPE15 (for corr. err.)

2 – if Sum Rules TAPE3 was created

- two separate stages:

1. the “diagonal”, or uncorrelated errors (calculated individually for each matrix element) and write them on TAPE15

**0 MS MEND 0 0 RMAX**

2. the “overall”, or correlated errors (the total errors which are the widths of projections on each matrix element’s axis of the minimum at the  $\chi^2 = \chi^2 + 1$  level). (**CONT SMR, for Sum Rules**). TAPE15 must be included as an input, TAPE3 will contain the output of OP,ERRO for program SIGMA (ATTENTION!!)

**1 MS MEND 1 1 RMAX**