MonteCarlo simulation of intermultiplet transitions in Pr

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Aim:

Project an High Inelastic Neutron Scattering experiment in the eV range energy on Prasodimio (Pr)

Monte Carlo simulation code give a prediction about the performance of the particular spectrometer before the realization of the experiment to organized the correct set up.

In this particular case we want to study the intermultiplet transition of Pr (rare-earth metal).

Summary

- Intermultiplet transitions
    - The spin-orbit interaction
- Inelastic Neutron Scattering
    - VESUVIO spectrometer
- MonteCarlo simulation

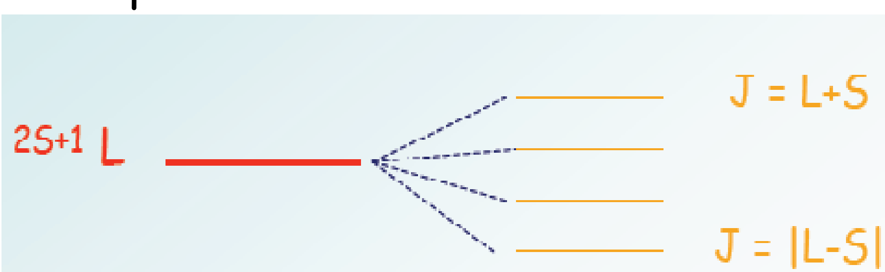
Intermultiplet transitions

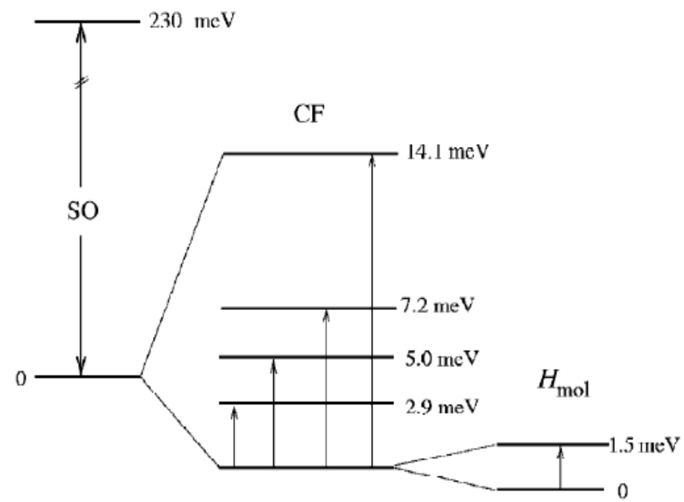
Hamiltonian of a system considering spin-orbit interaction is:

$$H = H_0 + H_{so}$$

$$H_{SO} = \sum_i \xi_i(r)\, \ell_i \cdot s_i = \zeta\, L \cdot S$$

where z is a radial integral of $\xi_i(r)$. The Spin-orbit interaction eliminates the degeneration of the ^{2S+1}L terms and generate J multiplets





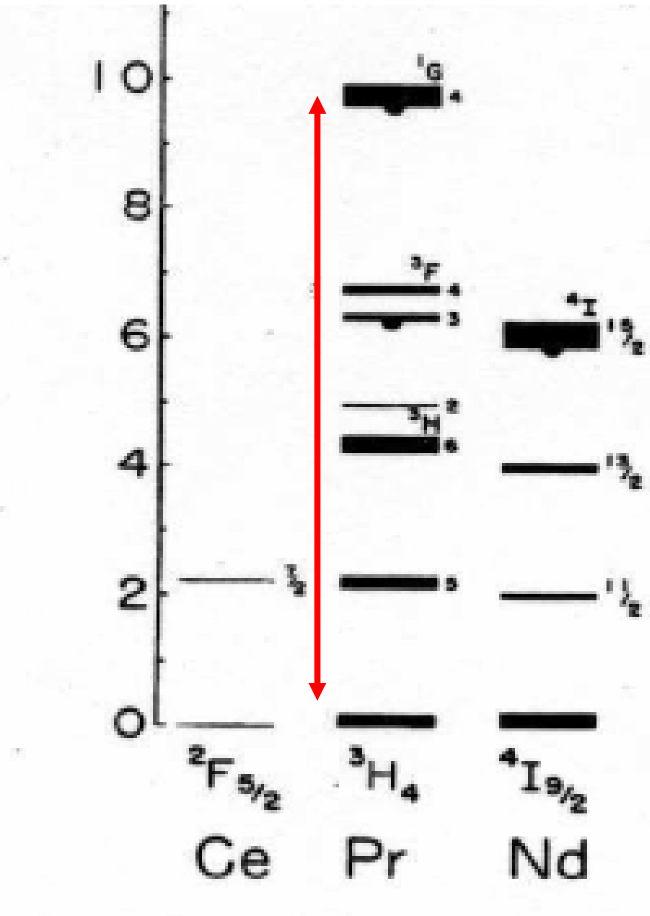
Typical splitting of levels in a rare earth system due to spin–orbit (SO), crystal-field (CF), and exchange interaction (H_{mol}). Scheme reproducing approximately the situation of Nd^{3+} ions in $NdCu_2$.

Intermultiplet transitions

Cross section:

$$\frac{d^2\sigma}{d\Omega dE_1} = \frac{k_1}{k_0}\sigma_n S_n(\mathrm{Q},\omega) + \frac{k_1}{k_0}\, r_0^2\, G(\mathrm{Q};\mu,\nu)\, \delta(\hbar\omega + E_\mu - E_\nu)$$

Intermultiplet transitions

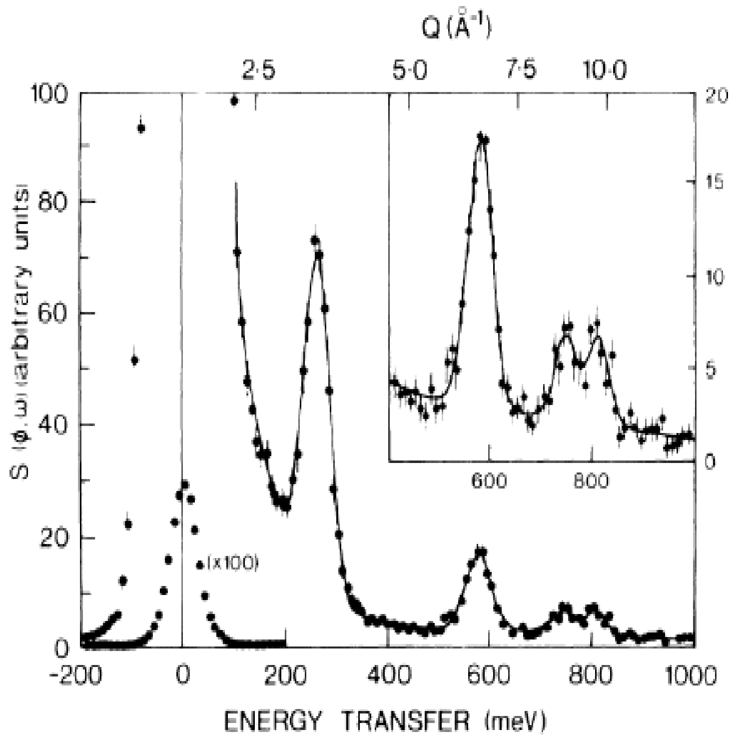


Transitions level of prasodimium.

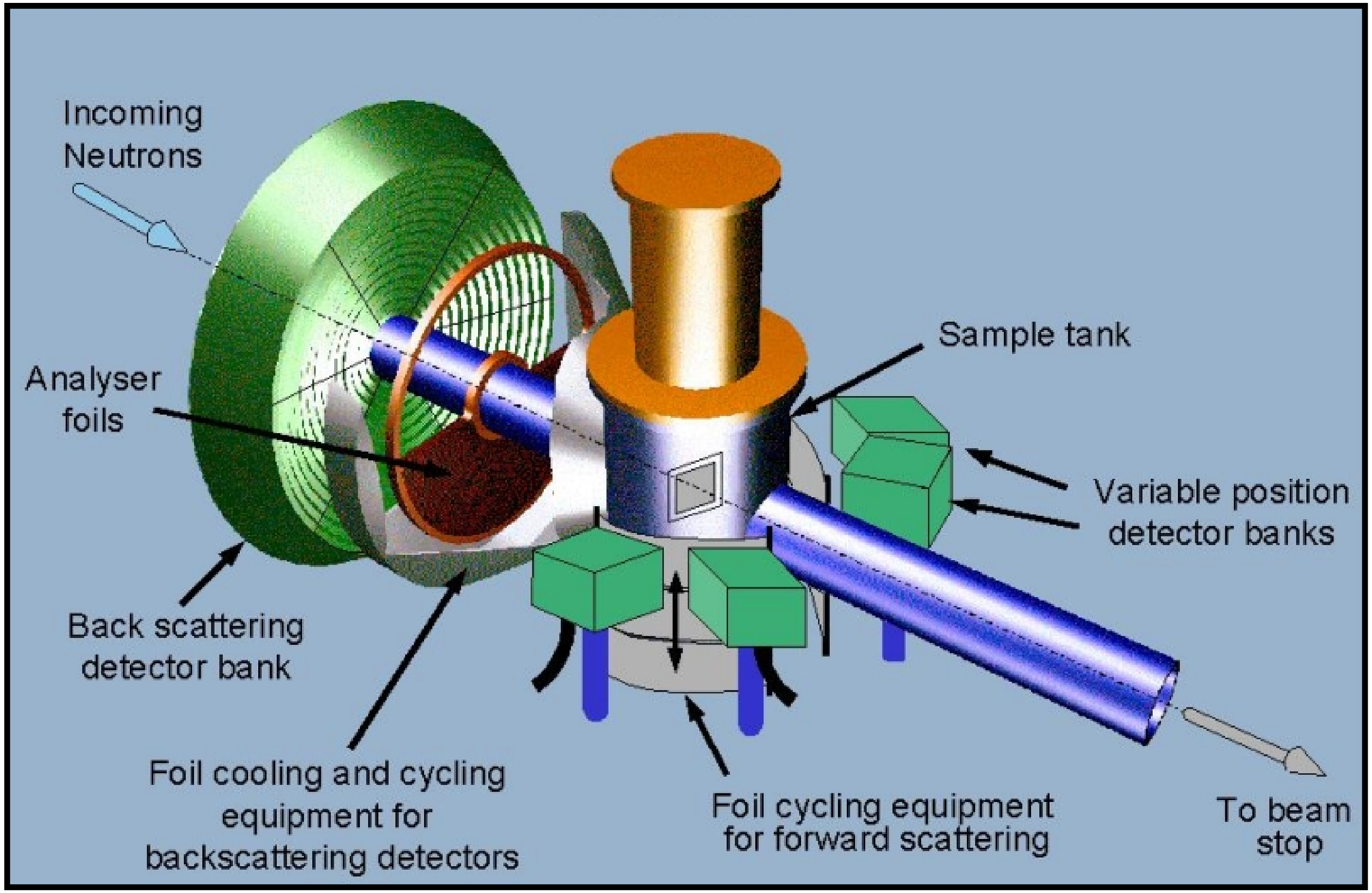
We want to observe the particular transition between $^3H_4$ and $^1G_4$

Prasodimium

Background: Intermultiplet transitions observed in metallic Pr in the range: $0 \leq \hbar\omega \leq 1600$ meV;$1 \leq Q \leq 15$ $\dot{A}^{-1}$; (A.D. Taylor et al., PRL, 61, 1309 (1988)). Transition $^3H_4 \rightarrow ^1 G_4$ @1170 meV was not observed.

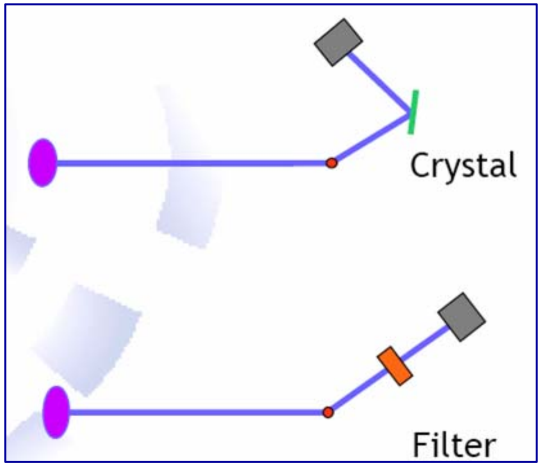


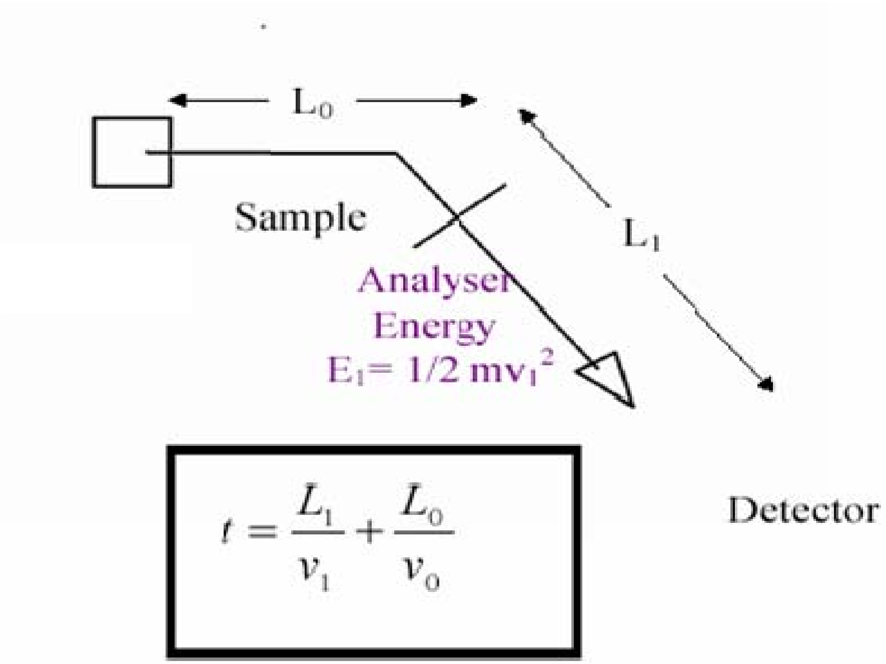
Vesuvio


Incoming Neutrons
Sample tank
Analyser foils
Variable position detector banks
Back scattering detector bank
Foil cooling and cycling equipment for backscattering detectors
Foil cycling equipment for forward scattering
To beam stop

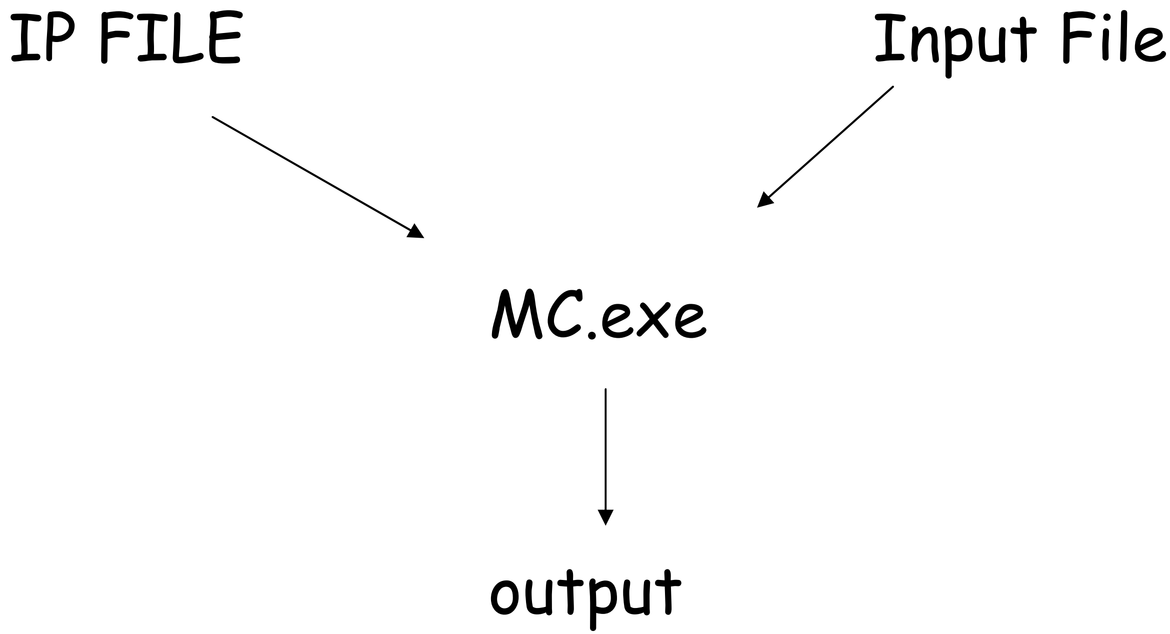
Time-of-Flight technique (T.O.F.)

- <u>Inverse geometry</u>
  (final energy selection)





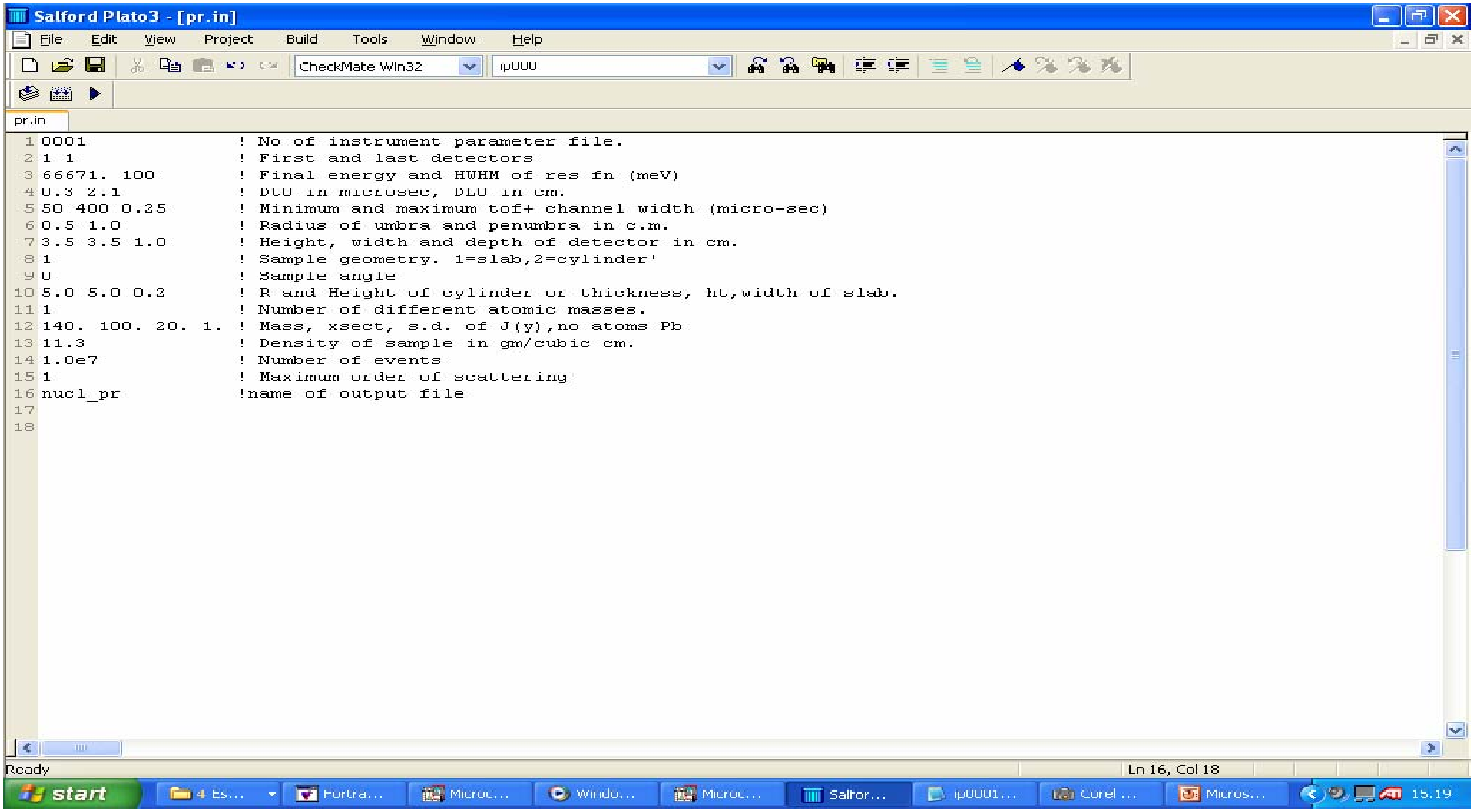
MonteCarlo Simulation



Instrument Parameters File

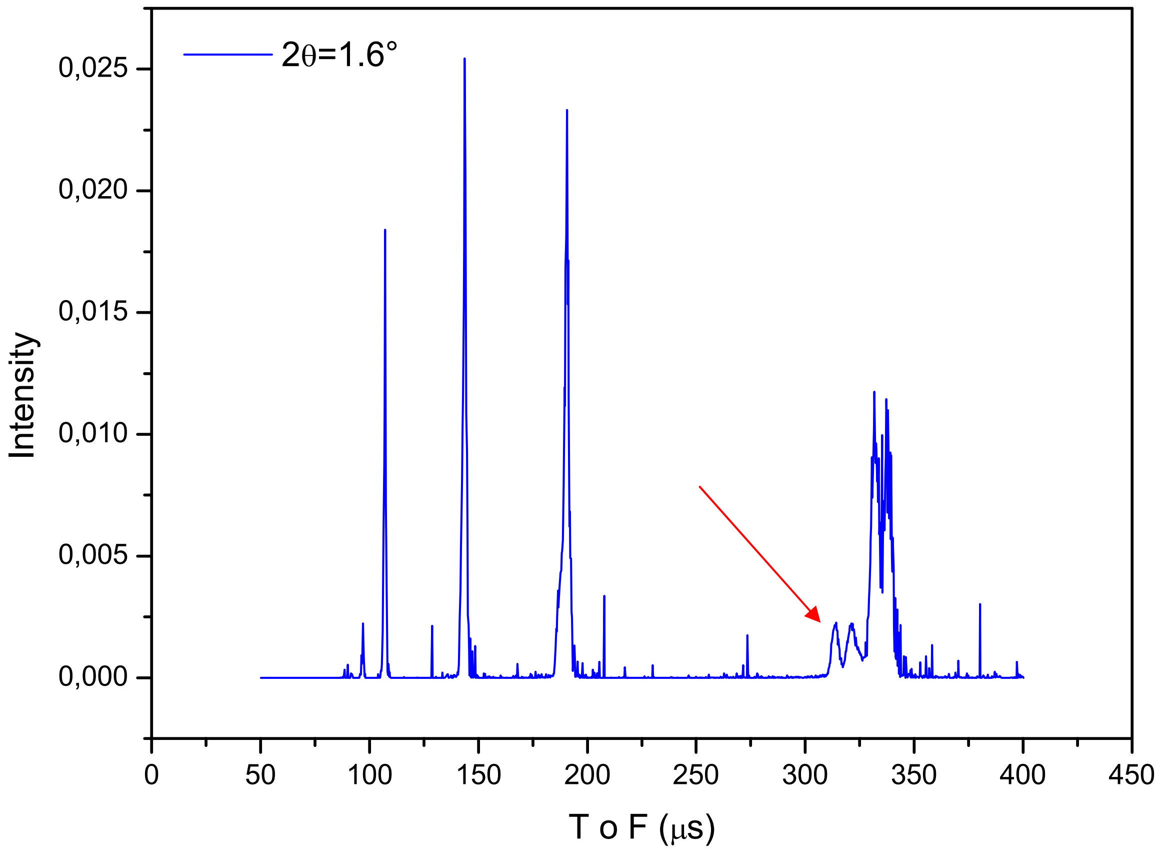
1	1.60	-5.5599999E-02	11.05500	1.01395000
2	2.00	-6.9100000E-02	11.05500	1.013
3	2.50	-2.3499999E-02	11.05500	1.013
4	3.00	-0.1553000	11.05500	1.013
5	-40.80000	-0.1629000	11.05500	0.6845000
6	-42.87000	-0.1137000	11.05500	0.6842000
7	-44.96000	-0.1874000	11.05500	0.6878000
8	-47.08000	-0.1999000	11.05500	0.6903000
9	-51.78000	-0.1767000	11.05500	0.6876000
10	-53.90000	-0.1103000	11.05500	0.6816000
11	-56.01000	-0.1802000	11.05500	0.6802000
12	-57.98000	-0.1244000	11.05500	0.6790000
13	-60.12000	1.3600000E-02	11.05500	0.6702000
14	-62.22000	-0.1458000	11.05500	0.6788000
15	-64.26000	-7.2700001E-02	11.05500	0.6803000
16	-66.27000	-0.1903000	11.05500	0.6874000
17	67.00000	-0.2220000	11.05500	0.7048000
18	65.36000	-0.1317000	11.05500	0.6925000
19	63.34000	-0.1028000	11.05500	0.6880000
20	61.28000	-0.1076000	11.05500	0.6889000
21	59.27000	-7.0900001E-02	11.05500	0.6803000
22	57.23000	-0.2223000	11.05500	0.6918000
23	55.13000	-5.8400001E-02	11.05500	0.6798000
24	53.06000	-0.2826000	11.05500	0.6932000
25	48.10000	2.0000000E-02	11.05500	0.6855000
26	46.16000	-0.1973000	11.05500	0.6932000
27	44.08000	-0.1922000	11.05500	0.6873000
28	41.92000	8.9599997E-02	11.05500	0.6687000
29	39.85000	-3.3599999E-02	11.05500	0.6745000
30	37.85000	-0.1995000	11.05500	0.6849000
31	35.76000	-0.1995000	11.05500	0.6849000
32	33.71000	-0.2554000	11.05500	0.6908000

Input File

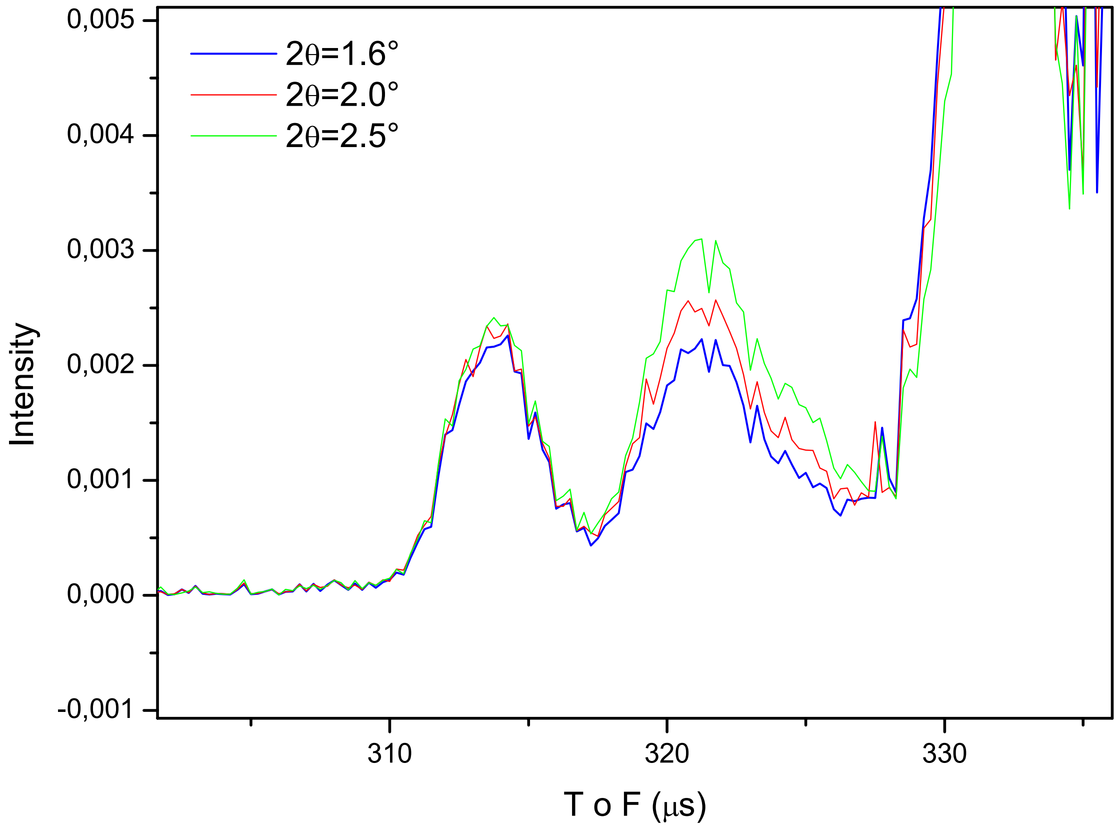


```
0001                  ! No of instrument parameter file.
1 1                   ! First and last detectors
66671. 100            ! Final energy and HWHM of res fn (meV)
0.3 2.1               ! Dt0 in microsec, DL0 in cm.
50 400 0.25           ! Minimum and maximum tof+ channel width (micro-sec)
0.5 1.0               ! Radius of umbra and penumbra in c.m.
3.5 3.5 1.0           ! Height, width and depth of detector in cm.
1                     ! Sample geometry. 1=slab,2=cylinder'
0                     ! Sample angle
5.0 5.0 0.2           ! R and Height of cylinder or thickness, ht,width of slab.
1                     ! Number of different atomic masses.
140. 100. 20. 1.      ! Mass, xsect, s.d. of J(y),no atoms Pb
11.3                  ! Density of sample in gm/cubic cm.
1.0e7                 ! Number of events
1                     ! Maximum order of scattering
nucl_pr               !name of output file
```

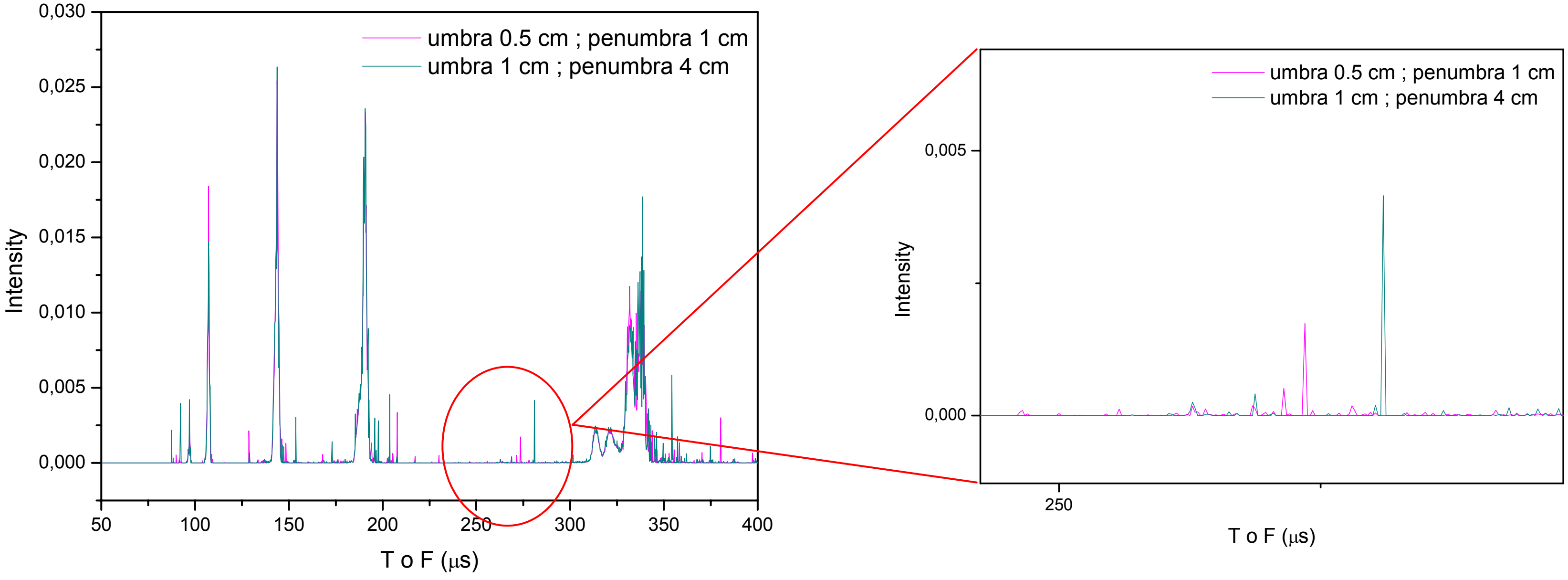
MonteCarlo Simulation



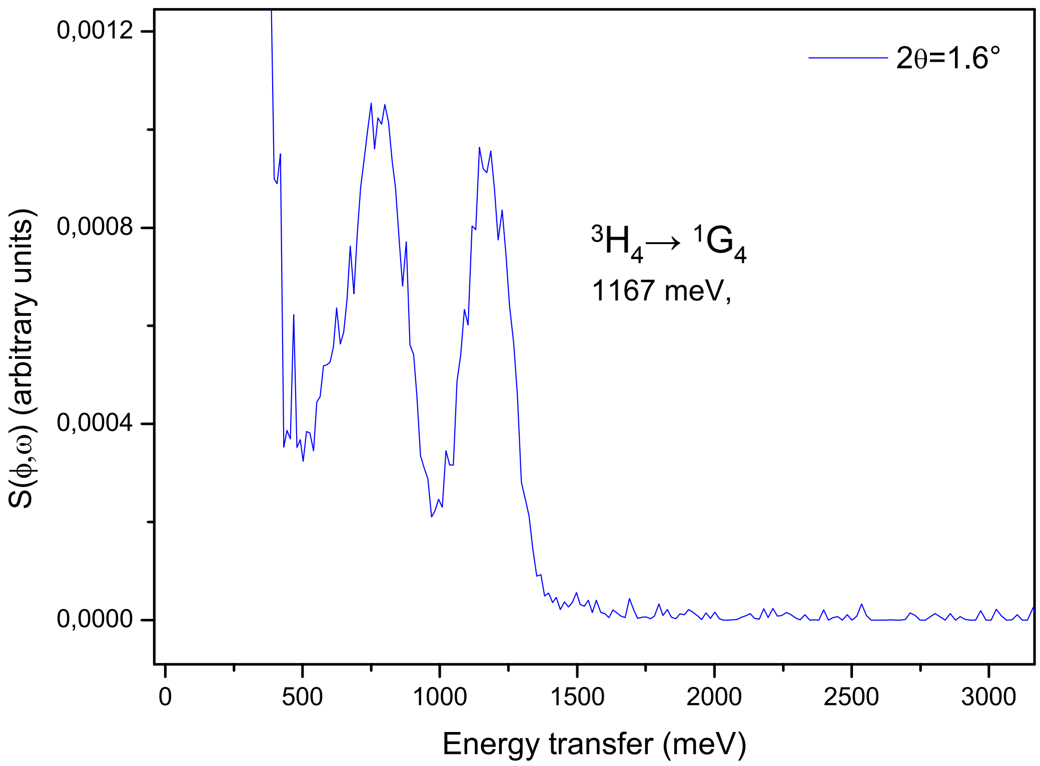
MonteCarlo Simulation



MonteCarlo Simulation



MonteCarlo Simulation



Conclusion

- Observation of intermultiplet transitions
- High Inelastic Neutron Scattering
- MonteCarlo Simulation in Pr