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BY DOPPLER BROADENING LINESHAPE ANALYSIS

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LINESHAPE ANALYSIS

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ABSTRACT

A program for the analysis of the dopplered gamma lineshape is described. The program calculates the lineshape and the Doppler-shift attenuation factor for a dopplered gamma line resulting from the emission of recoiling ions produced in a reaction on a thin layer and slowing down in a stopping material. Nuclear lifetimes are extracted by a best fit of the experimental line (chisquare criterion). Spreading in the initial velocity of the recoiling ions, finite detection geometry, angular efficiency of the detector, angular distribution of gamma rays and feeding from higher levels are taken into account in the code.

PROGRAM SUMMARY

Peculiarities of the physical problem

The program calculates the lineshape and the Doppler-shift attenuation factor $F(\tau)$ for a dopplered gamma line resulting from the emission of recoiling ions, produced in a reaction on a thin target and slowing down in a stopping material.

The main peculiarities taken into account by the code are:

- the kinematical spread in the initial velocity of the recoiling nuclei;
- the limitation in the initial velocity range of the recoiling ions for particle-gamma coincidences;
- the finite detection geometry;
- the energy response (gaussian) and angular efficiency of the Ge(Li) detector;
- the angular distribution of emitted gamma rays;
- the feeding from a level of known lifetime and intensity;
- the angular distribution of the recoiling nuclei assumed isotropic in the center of mass.

Peculiarities of the code

Title of program: NADOP

Computer and operating system: HP1000 - RTE VI

Language: FORTRAN 77

High speed storage required: 32 Kwords

Number of bits in a word: 16

Peripheral used: 1 disk pack and 1 magnetic tape (optional).

1. - INTRODUCTION

The Doppler shift attenuation method has been widely used for the extraction of nuclear lifetimes.

In recent years lifetime measurements by the DSA method using heavy ion induced reactions on light nuclei have provided a substantial improvement in precision and accuracy with respect to the conventional "direct" reactions. In this case, the slowing down process takes place mostly at high velocities, where experimental data on the stopping power are available with good accuracy and where the importance of the Doppler shift effect allows an accurate lineshape analysis. On the other hand the theoretical lineshape calculation has to be carried out taking into account the details of the decay process of the recoiling nuclei, in order to obtain good fits to the data.

We present here a computer code which performs the analysis of the Doppler broadened gamma line, taking into account:

- the kinematical spread in the initial velocity of the recoiling nuclei;
- the angular distribution of gamma-rays and the angular dependence of the detector efficiency;
- the response function of the detector;
- the feeding from high-lying levels.

The method of analysis will be described in Section 2. In Sections 3 and 4 a description of the code and some results will be given.

2. - METHOD OF ANALYSIS

The lifetime value τ is extracted by a least squares fit of the theoretical lineshape to the background subtracted experimental data. For a given τ value the number of recoiling nuclei deexciting at velocity $V=v/v_i$, where v_i is the initial velocity, is

$$\frac{dN}{dV} = \frac{e}{\tau} \frac{-t(V)}{dV} dt \quad (1)$$

normalizing to 1 the total number of recoiling nuclei. The function $t(V)$ is obtained by integration of the usual parametrization of the stopping power:

$$-\frac{MdV}{\rho dt} = \begin{cases} K_n \left(\frac{V}{V_0}\right)^{-1} + K_e \left(\frac{V}{V_0}\right) - K_3 \left(\frac{V}{V_0}\right)^3 & \text{for } 0 < \frac{V}{V_0} \leq \frac{V_c}{V_0} \\ A + B \left(\frac{V}{V_0}\right) - C \left(\frac{V}{V_0}\right)^2 & \text{for } \frac{V_c}{V_0} \leq \frac{V}{V_0} \leq 1 \end{cases} \quad (2)$$

where $V_0 = v_0/v_i = c/137 v_i$, M is the ion mass and ρ is the slowing down material density. This yields:

$$\frac{dN}{dV} = \begin{cases} \frac{x(\gamma_+ - \gamma_-)}{(\gamma_+ + V)^2} \left(\frac{1 + \gamma_+}{1 + \gamma_-} \right)^x \left(\frac{\gamma_- + V}{\gamma_+ + V} \right)^{x-1} & \text{for } V_c \leq V \leq 1 \\ (\beta_-^2 + \beta_+^2) V_o^2 \left[\frac{(V_c + \gamma_-)(1 + \gamma_+)}{(V_c + \gamma_+)(1 + \gamma_-)} \right]^x \left(\frac{V_c^2 - V_o^2 \beta_+^2}{V_c^2 + V_o^2 \beta_-^2} \right)^{z/2} z V \frac{(V^2 + V_o^2 \beta_-^2)^{\frac{1}{2}z-1}}{(V^2 - V_o^2 \beta_+^2)^{\frac{1}{2}z+1}} & \text{for } 0 < V \leq V_c \end{cases} \quad (3)$$

where $x = Mv_o / Q\tau$ and $z = Mv_o / K\tau$.

The quantities $Q, K, \gamma_+, \gamma_-, \beta_+, \beta_-$, are expressed as functions of the slowing down coefficients of Eq. (2), as follows (Refs. (1) and (2)):

$$\begin{aligned} Q^2 &= B^2 + 4 AC & K^2 &= K_e^2 + 4 K_n K_3 \\ \gamma_{\pm} &= \frac{-V_o}{2C} (B \pm Q) & \beta_{\pm}^2 &= \frac{K \pm K_e}{2 K_3} \end{aligned}$$

The number of nuclei deexciting at rest $N(V=0)$ defined as

$$N(V=0) = 1 - \lim_{V \rightarrow 0} \int_V^1 \frac{dN}{dV} dV ,$$

is given by the following expression:

$$N(V=0) = \left[\frac{(V_c + \gamma_-)(1 + \gamma_+)}{(V_c + \gamma_+)(1 + \gamma_-)} \right]^x \cdot \left[\frac{(V_o^2 \beta_+^2 - V_c^2) \beta_-^2}{(V_o^2 \beta_-^2 + V_c^2) \beta_+^2} \right]^{z/2} \quad (4)$$

In the program the number of nuclei deexciting at velocities $V < V_c$ is computed in terms of the parameters γ_i and C_i , used in Ref. (1) and defined as:

$$\gamma_i = \frac{1}{V_o \beta_-} \quad C_i = \frac{1 + \gamma_i^{-2}}{V_o^2 \beta_+^2 - 1}$$

The number of the emitted gamma-rays for each energy value E , in the range of the Doppler shifted pattern, is calculated by integration of the function dN/dV weighted by the detection efficiency $\varepsilon(\theta)$ and the gamma-rays angular distribution $W(\theta)$, utilizing the following expression:

$$\frac{dN}{dE} = \int_{V_{\min}}^{V_{\max}} \frac{dN}{dV} W(\cos \theta(V)) \varepsilon(\theta(V)) J(V) dV \quad (5)$$

with

$$V_{\min} = (E - E_o) / E_o \quad \text{and} \quad V_{\max} = (E - E_o) / (E_o \cos \theta_{\max})$$

where E_o is the energy of the gamma-ray emitted by nuclei at rest and θ_{\max} is the semiangle subtended by the detector. The Jacobian $J(V)$ is given by $E_o V v_{in} / c$. The number of the gamma-rays of energy E_o is given by

$$N(E_o) = \frac{N(V=0)}{2} \int_0^{\theta_{\max}} W(\theta) \varepsilon(\theta) \sin \theta d\theta \quad (6)$$

In order to take into account the spread in the initial velocity arising from the reaction kinematics, the theoretical lineshape is obtained by a convolution of the expressions (5) and (6) with a distribution function of the initial velocities calculated assuming an isotropic angular distribution of the recoiling ions in the center of mass system. In a similar way the distribution of the initial velocities due to the energy loss in the target region can be taken into account.

The resulting lineshape is finally convoluted with the intrinsic response function $R(E-E')$ of the detector (taken as a gaussian function):

$$\frac{dN}{dE} = \int_0^{\infty} \frac{dN}{dE'} R(E-E') dE' \quad (7)$$

When the level under investigation is populated by a level of known lifetime τ_f with feeding intensity b , the expression (1) is replaced by:

$$\frac{dN}{dV} = \left[\frac{e^{-t(V)/\tau}}{\tau} \left(1 - \frac{b}{1-\tau/\tau_f}\right) + \frac{e^{-t(V)/\tau_f}}{\tau_f} \frac{b}{1-\tau/\tau_f} \right] \frac{dt}{dV} \quad (8)$$

Moreover the program calculates the Doppler-shift attenuation factor $F(\tau)$ for both the theoretical and experimental lines following the expression:

$$F(\tau) = \frac{\langle E \rangle - E_o}{E_{\max} - E_o}$$

where $\langle E \rangle$ is the centroid energy of the detected gamma rays and E_{\max} is the energy of the gamma line emitted at maximum velocity of the recoiling nuclei.

3. - CODE DESCRIPTION

Following the method described in the previous Section, a code was written which performs the various operations.

The program consists of a main program NADOP and 8 subroutines. Fig. 1 shows the block diagram of the program organization. In the following a description of the main program and of the subroutines, in the order as they are called by the main, is given.

NADOP

The main program NADOP is capable of computing the gamma dopplered lineshape as a function of lifetime (TAU). A χ^2 value from the difference between the background subtracted experimental lineshape and the theoretical one, normalized to the total experimental area, is calculated. Starting with a TAU value chosen by the user the program calculates the χ^2 function increasing or decreasing TAU iteratively with a constant step DTAU till a minimum is detected. The final lifetime and related error are extracted by approximating the χ^2 function with a parabola in the vicinity of the minimum.

ENL2

SPECT

QINEM

ENNE1

ENNE2

ENNE1

ENNE1

ADEC

GAUSCO

GAUMI

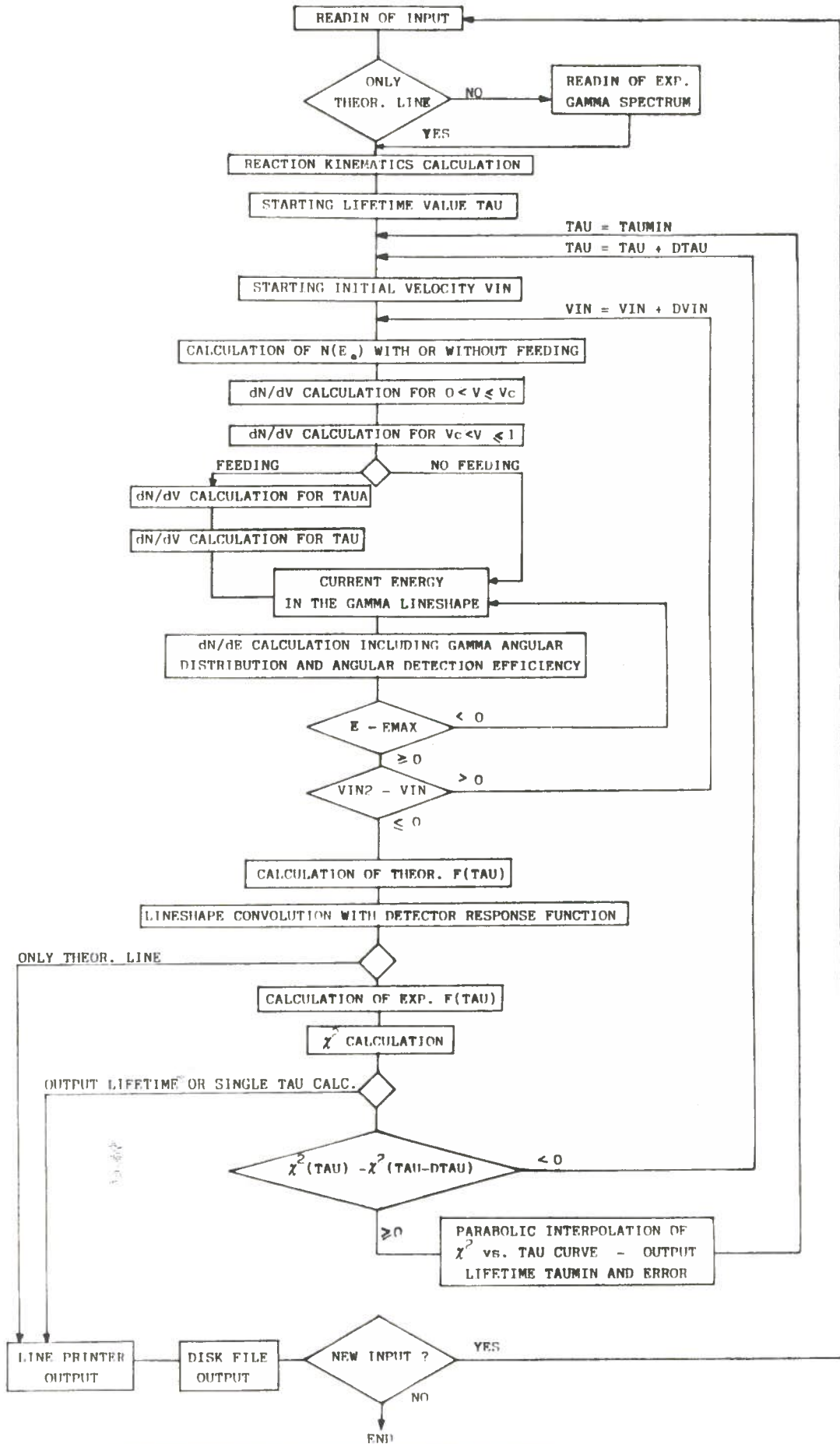


FIG. 1 - Block diagram of the program organization.

Moreover, the $F(\text{TAU})$ function is calculated relative to the experimental and theoretical lineshapes following Eq. (9).

The range of the initial velocities (VIN2-VIN1) of the recoiling nuclei is divided in NVIN intervals and the calculation of the theoretical lineshape is carried out by superposition of the single lineshapes relative to the mean initial velocity in each interval. For each value of the initial velocity the parameters employed for the calculation of the single lineshape are evaluated and the number of the detected gamma rays emitted by the recoiling ions at rest is calculated by the expression (6).

The evaluation of the single line is performed with an energy step (DE) equal to the experimental energy conversion or scaling it by a factor IDE , assigning to each interval the energy average value in the interval.

The choice of the energy step should come out from a compromise between the need of an accurate description of the theoretical lineshape and the computer time needed to perform the calculation. In any case the energy step should be much smaller than the experimental energy resolution and should yield an area under the theoretical lineshape very close to the absolute efficiency.

In the case a value of $\text{IDE} > 1$ is employed, the program groups the values of the theoretical lineshape for the comparison with the experimental ones.

The lineshape calculation can be performed taking into account the contribution to the population of the level under study by a level at higher excitation energy of known lifetime (TAUA) and branching using the expression (8) instead of (1).

Subroutine INIZ

INIZ reads all the parameters and options needed to perform the calculation.

A disk file is utilized to provide the values of the parameters regarding: reaction, level under study, detection geometry, stopping material, slowing down process, energy calibration, experimental resolution and channel regions relative to the dopplered gamma-line and background. Data are displayed to the user who can modify them.

The file structure, together with the definition of the input parameters, is given in Table 1.

The remaining parameters, to be supplied by keyboard, are: the starting value of the lifetime (TAU), the step of variation in the lifetime (DTAU), the number of intervals in the initial velocity range (NVIN) and the energy conversion scaling factor (IDE).

Moreover, the user is requested to reply to the following questions:

- 1) calculation of the theoretical lineshape for a single lifetime without reading the experimental spectrum;
- 2) comparison between the theoretical and experimental lineshapes for a single lifetime;
- 3) calculation including the contribution of the population of the level under study by a level at higher excitation energy. In this case lifetime and branching of the feeding level should be supplied to the program;
- 4) calculation for the case of particle-gamma coincidences for which the range of the initial velocities is requested;
- 5) storage on disk files of the theoretical and experimental lineshapes and choice between two different formats (binary or ASCII type files).

TABLE I - Description of input disk file parameters.

1	TI	Projectile symbol	
2	TT	Target symbol	
3	TP	Ejectile symbol	
4	FCUS	Slowing down material symbol	
5	NI	Projectile mass	
6	NT	Target mass	
7	NP	Ejectile mass	
8	EIL	Laboratory projectile energy	(MeV)
9	Q ϕ	Reaction Q-value	(MeV)
10	EX	Initial level energy	(MeV)
11	EY	Final level energy	(MeV)
12	DBR	Detector target distance	(cm)
13	DRR	Detector diameter	(cm)
14	RIN	Internal detector radius	(cm)
15	XL	Detector length	(cm)
16	CA	Photoelectric absorption coefficient	(cm ⁻¹)
17	J ϕ	J ₀ integral	
18	J ₂	J ₂ integral	
19	A ₂	Gamma angular distribution coefficient	
20	SIG	Detector resolution	(keV)
21	E ϕ	Energy intercept	(keV)
22	DE	Linear energy conversion	(keV/chan)
23	CIN	Gamma line initial channel	
24	NCAN	Gamma line number of channels	
25	ICA1	Left background initial channel	
26	ICA2	Left background final channel	
27	ICA3	Right background initial channel	
28	ICA4	Right background final channel	
29	EQ	Quadratic energy conversion	(keV/chan ²)
30	AKN	Slowing down parameter K _n	} (x)
31	AKE	Slowing down parameter K _e	
32	AK3	Slowing down parameter K ₃	
33	ACO	Slowing down parameter V _c	
34	A	Slowing down parameter A	
35	B	Slowing down parameter B	
36	C	Slowing down parameter C	
37	R ϕ	Slowing down material density	(1000 g/cm ³)

(x) see Eq. (2) for symbols.

Subroutine SPECT

SPECT reads the experimental gamma-ray spectrum from disk or magnetic tape and computes the background subtracted line.

Subroutine CINEM

CINEM calculated the reaction kinematics, in particular the range of the initial velocities of the recoiling nuclei.

Subroutine ENNE1 and ENNE2

These subroutines compute the dN/dV function of the slowing down nuclei in 1000 steps from the initial velocity till rest using the expression (3). ENNE1 and ENNE2 refer to velocities $1 \leq V \leq V_c$ and $V_c \geq V > 0$ respectively. These subroutines are called for NVIN initial velocities.

Subroutine ADEC

Following the expression (5), this subroutine calculates the values of the dN/dE function for a given energy. It carries out a numerical integration of the weighted dN/dV function in the velocity range which, due to the finite detection geometry, contributes to the number of gamma rays of energy E.

Subroutine GAUSCO

GAUSCO realizes the convolution of the dN/dE function with the response function of the detector, assumed to be gaussian, following the expression (7). The energy step in the calculation is the same used in the evaluation of the single lineshape.

Subroutine TAUMI

This subroutine performs the interpolation of the χ^2 vs TAU curve by means of a parabolic function.

The lifetime corresponding to the minimum of the function represents the best fitted lifetime. The error on the lifetime is calculated in terms of the curvature of the parabola at the vertex. The lineshape for the output lifetime is finally calculated in the main program.

4. - DIMENSION RESTRICTIONS

- The spectrum to be read must contain less than 2048 channels;
- The spectrum region to be fitted must contain less than 128 channels (NCAN);
- The maximum number of steps in lifetime for the minimum χ^2 search is 100 (the user is warned by a message when no minimum has been found);
- The maximum number of points describing the theoretical lineshape is 500.

From the above restrictions, the energy scaling factor IDE must be less than $500/NCAN$.

5. - RESULTS

The program NADOP has been used to extract the lifetimes of nine low-lying levels in ^{18}F , populated via the reaction $^3\text{He}(^{16}\text{O},\text{p})^{18}\text{F}$ using ^3He implanted targets (Refs. (3) and (4)). Lifetime values from 5.8 to 0.02 ps (χ_n^2 values of 1.5 to 0.7) and upper limits of 4 and 8 fs were found.

As an example we will discuss here the lineshape analysis of the 660 keV gamma line deexciting the 1.7 MeV level. Such an analysis carried out on data taken at 21 MeV oxygen beam on Al backing both in singles and in coincidence with the protons, shows the influence on the lifetime of the feeding from higher levels.

In the case of singles data, the initial velocity range was $v/c = (4.47 \pm 0.48)\%$ splitted, for the purpose of the analysis, in $N_{\text{VIN}} = 5$ intervals. This value was found to be sufficient to reproduce quite well the slope of the gamma line in the totally Doppler shifted energy region. Being the energy resolution $\text{SIG} = 1.90$ keV and the energy conversion $\text{DE} = 0.719$ keV/channel, a scaling factor $\text{IDE} = 3$ was chosen, which provided an area under the theoretical lineshape equal to the absolute efficiency within 0.2%. Starting the χ^2 minimum search with an initial value of the lifetime of 0.9 ps and a step of 0.05 ps, a final value of 1.18 ± 0.02 ps with a normalized $\chi_n^2 = 1.1$ was obtained with a CPU time of 33 min (Fig. 2).

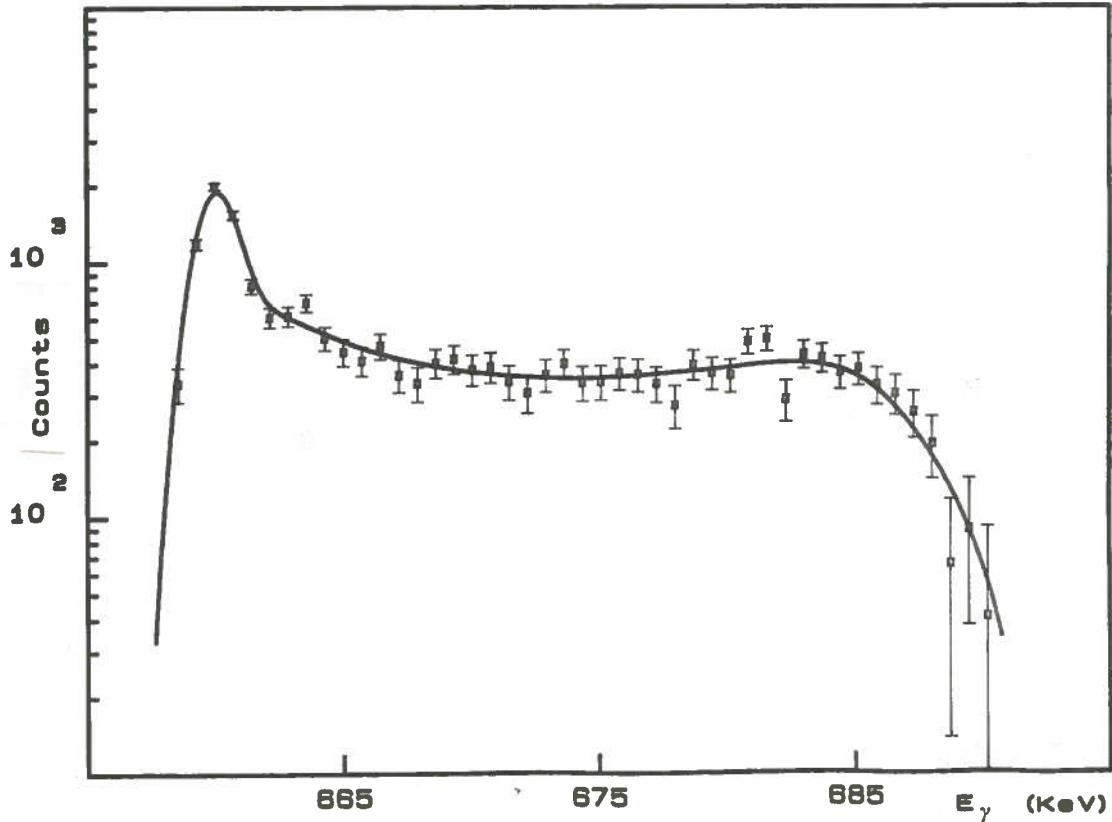


FIG. 2 - Background-subtracted Doppler γ -ray pattern of the 1.70-1.04 MeV transition in ^{18}F . Solid line represents the best fit to the data without feeding.

A best fit of equivalent quality (Fig. 3) was obtained using the same input data, except for the additional condition of a 30% feeding intensity from a higher level with a lifetime of 0.6 ps. The resulting value of the lifetime for the 1.7 MeV level was of 0.97 ± 0.02 ps with a $\chi_n^2 = 1.5$.

It turns out that the inclusion of a feeding can lead to undistinguishable fits with respect to the case of no feeding in which a longer apparent lifetime is extracted. The presence of the feeding effect in the population of the 1.7 MeV level is confirmed by the analysis of the coincidence data. Such an

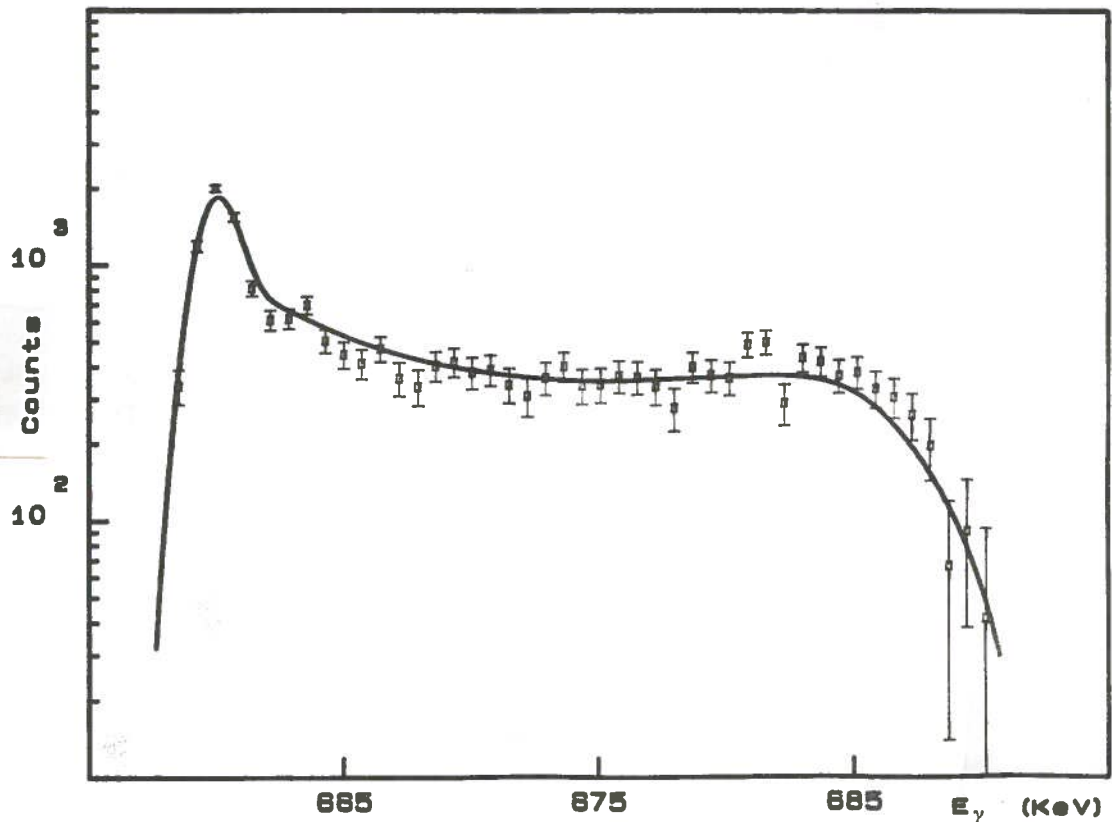


FIG. 3 - Background-subtracted Doppler γ -ray pattern of the 1.70-1.04 MeV transition in ^{18}F . Solid line represents the best fit to the data with a 30% feeding intensity from a level of 0.6 ps lifetime.

analysis was performed with the same input parameters as in the case of single data with the exception of the NVIN parameter which was set equal to 1, being the initial velocity range reduced to $v/c=(3.995 \pm 0.005)\%$ by the coincidence requirement. The resulting lifetime value of 0.93 ± 0.02 ps with a $\chi_n^2=1.2$ agrees very well with the one obtained by the analysis of the single data with feeding inclusion.

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