Theoretical predictions on the air-fluorescence yield

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Fourth air fluorescence workshop
Prague - Pruhonice May 2006

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Introduction

- Fluorescence yield is a key parameter for a reliable calibration of fluorescence detectors (HiRes, AUGER, EUSO, OWL)
- Lab measurements needed (FLASH, AIRFLY, Karlsruhe, Paris, MACFLY, LIP, UCM,...)

This work

Fluorescence yield can be **calculated** from the various **cross sections** involved in the excitation / de-excitation processes.

Objectives

Predictions on:

- Absolute value of fluorescence yield
- Energy dependence of the fluorescence yield
- Effects of environmental parameters
- Fluorescence yield versus deposited energy

Very important !!

Particular attention has to be paid to **secondary electrons** ejected in molecular ionizations.

more details in:

The yield of air fluorescence induced by electrons

F. Arqueros ,F. Blanco, A. Castellanos, M. Ortiz, J. Rosado

submitted to Astroparticle Physics and available in:
arXiv:astro-ph/0604498 v1 24 Apr 2006

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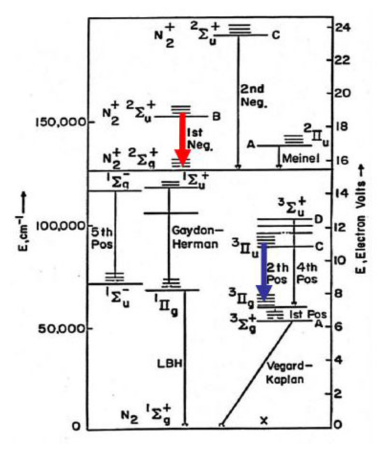
Spectral range of interest - Molecular levels involved



Spectral range: 300 - 420 nm

1N First Negative System of N_2^+
$(B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+)$

2P Second Positive System of N_2
$(C^3\Pi_u \rightarrow B^3\Pi_g)$

Fluorescence yield $\varepsilon_{vv'}$ at very low pressure

$\varepsilon_{vv'}$ = number of fluorescence v-v' photons emitted per electron and meter.

$\varepsilon_{vv'}$ is fully determined by the *optical cross section* $\sigma_{vv'}$

$$\varepsilon_{vv'} = N\sigma_{vv'} \tag{1}$$

Excitation cross section σ_v / Franck-Condon factors $q_{X\to v}$

$$\sigma_{vv'} = \sigma_v B^{vv'} \ , \ \sigma_v \propto q_{X\to v} \tag{2}$$

$$\frac{\varepsilon_{vv'}}{\varepsilon_{00}} = \frac{q_{X\to v}}{q_{X\to 0}} \frac{B^{vv'}}{B^{00}} \tag{3}$$

Collisional quenching

a) reduces fluorescence yield

$$\varepsilon_{vv'}(P) = N\sigma_{vv'} \frac{1}{1 + P/P'_v} \tag{4}$$

b) shortens fluorescence lifetime

$$\frac{1}{\tau^v(P)} = \frac{1}{\tau^v_r}(1 + \frac{P}{P'_v}) \tag{5}$$

Quenching effects are determined by a characteristic pressure P' given by the collisonal cross sections $(\sigma_{nn}, \sigma_{no}, ..etc.)$

$$P'_v = \frac{\sqrt{\pi M_n kT}}{4\tau_r}\{f_n\sigma_{nn} + f_o\sigma_{no}\sqrt{\frac{M_n + M_o}{2M_o}}\}^{-1}, \tag{6}$$

Secondary electrons

F. Blanco and F. Arqueros, Phys. Lett A 345 (2005) 355

Secondary excitations increase fluorescence emission

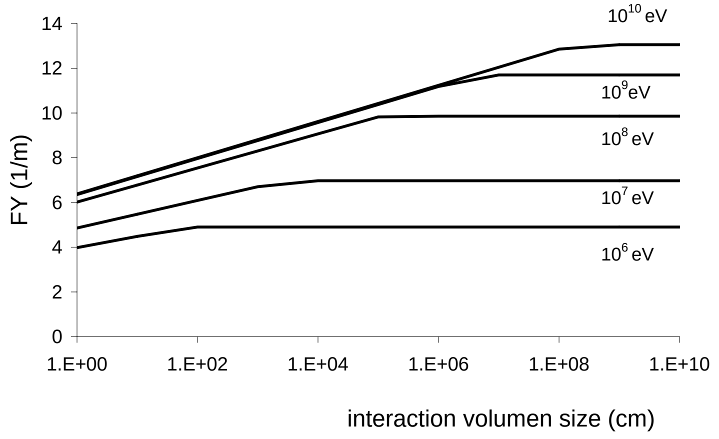
$$\sigma^{eff}_{vv'} = \sigma_{vv'}(E) + \alpha_{vv'}(E,P)\sigma_{ion}(E) \tag{7}$$

$\alpha_{vv'}$ has been calculated by means of a Monte Carlo simulation.

$$\alpha_{vv'}(E,P) = \min\{s_0 \ln \frac{P \times R}{s_1}, e_0 \ln \frac{E}{e_1}\} \tag{8}$$

Smooth dependence on P, E and the size of the interaction region R. More details will be published soon.

Results of our model



Fluorescence yield at high pressure

$$\varepsilon_{vv'}(P) = N\frac{1}{1+P/P'_v}\left\{\sigma_{vv'}(E)+\alpha_{vv'}(E,P)\sigma_{ion}(E)\right\} \tag{9}$$

- Collisional quenching (Stern-Volmer)
  - $\varepsilon_{vv'}/N$ decreases with pressure
  - Reciprocal lifetime $\propto$ pressure $\Rightarrow$ Safe procedure for P' measurement
- Fluorescence induced by secondary electrons (model)
  - $\varepsilon_{vv'}$ increases by a factor (smoothly dependent on P, E and R!!)
  - At high pressure: a) non-negligible correction for the 1N System. b) dominant contribution for the 2P System
  - Secondary electrons distort the $\varepsilon_{vv'}(P)$ function $\Rightarrow$ Caution!! Erroneous determination of P'??

Parameters of the model for secondary electrons

$$\alpha_{vv'}(E,P) = \min\{s_0 \ln \frac{P \times R}{s_1}, e_0 \ln \frac{E}{e_1}\} \tag{10}$$

	s_0	s_1 (hPa×cm)	e_0	e_1(eV)
1N (0-0)	$8.67 \cdot 10^{-3}$	$1.92 \cdot 10^{-2}$	$1.37 \cdot 10^{-2}$	73.7
2P (0-0)	$2.00 \cdot 10^{-3}$	$1.36 \cdot 10^{-5}$	$3.22 \cdot 10^{-3}$	0.942

Table 1.- *Values of the parameters for the most prominent bands of the 1N and 2P molecular systems.*

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Calculation ingredients

- Optical cross section for direct excitation $\sigma_{00}^{1N}(E)$ and $\sigma_{00}^{2P}(E)$ from experimental data (extrapolated to high energies)
- Ionization cross section $\sigma_{ion}(E)$ from experimental data (extrapolated to high energies).
- $\alpha_{00}(E, P, R)$ from MC calculation (model)
- Transition probabilities $B^{vv'}$ and Franck-Condon factors $q_{X\rightarrow v}$ from literature (theoretical values in agreement with experimental data)
- Experimental P' values.

Parameters

$R = 2.5$ cm

$T = 300$ K

eVs $< E <$ 100 GeV

1 hPa $< P <$ atmospheric pressure

The 1N system

Optical cross sections:
Cross section for the excitation to the $B^2\Sigma_u^+$ (N_2^+) level (also total ionization cross section σ_{ion}) follows the Born-Bethe law.

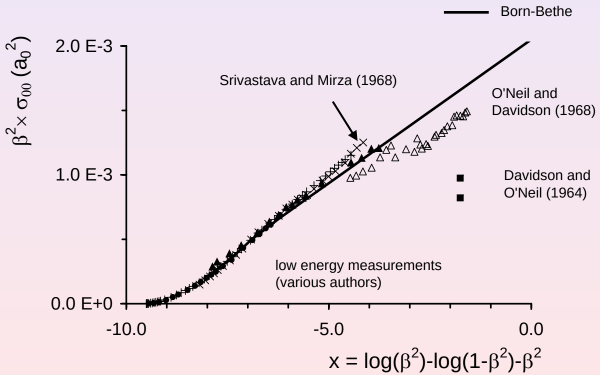
Born-Bethe with density correction

$$\sigma = \frac{A}{\beta^2}\{\ln C\beta^2 - \ln(1-\beta^2) - \beta^2 - \delta_F\}\,, \tag{11}$$

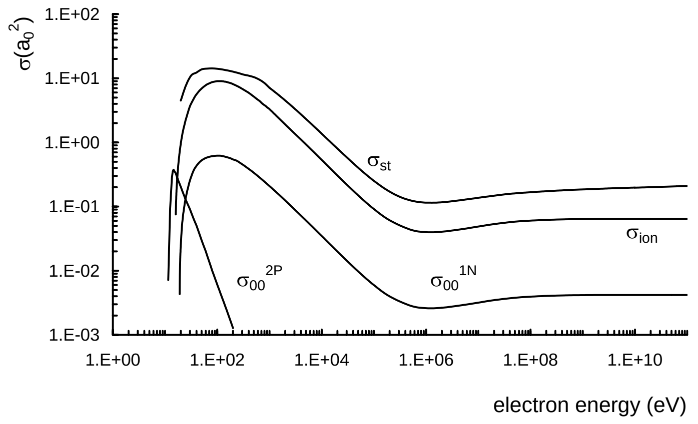
For small δ_F values (low pressure, low energy) the cross sections is linear in a Fano plot i.e. $\sigma\beta^2$ versus $x = \ln(\beta^2) - \ln(1-\beta^2) - \beta^2$

Experimental optical cross sections for the 1N system

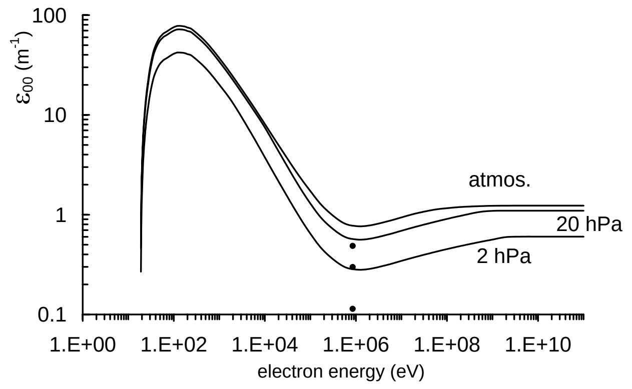
Fano plot for σ_{00} (391.4 nm)



Cross sections involved in the fluorescence emission

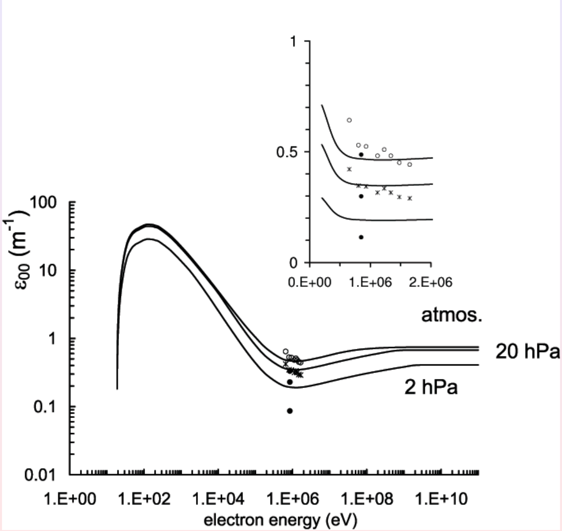


1N (391.2 nm) fluorescence yield for pure nitrogen



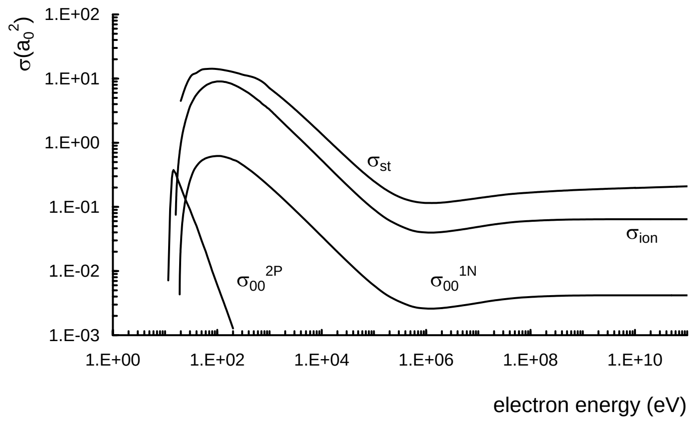
Our calculations (——), Nagano et al. (•)

1N (391.2 nm) fluorescence yield for dry air

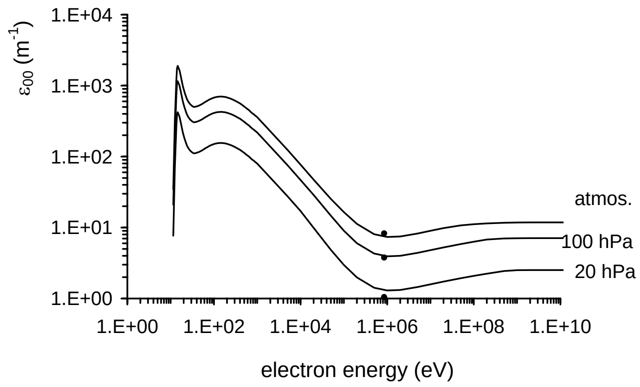


Our calculations (——)
Nagano et al. (•)
Hirsh et al. (⋆, ○)

The 2P System. 0-0 optical cross section

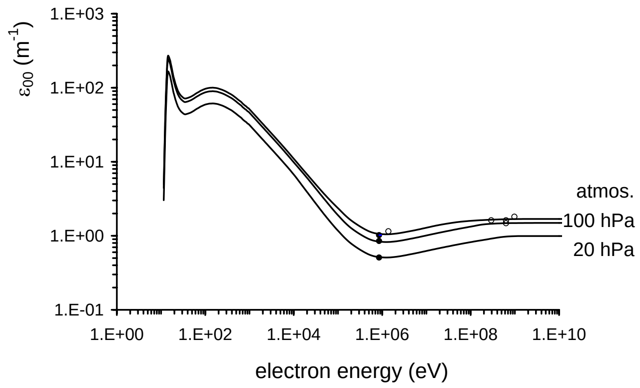


2P (337.0 nm) fluorescence yield for pure nitrogen



Our calculations (——), Nagano et al. (•)

2P (337.0 nm) fluorescence yield for dry air



Our calculations (——), Nagano et al. (●), Ueno - atmosph.pres. (○)

Total fluorescence yield

Total fluorescence yield

$$\varepsilon = \sum_{vv'} \varepsilon_{vv'}^{1N} + \sum_{vv'} \varepsilon_{vv'}^{2P} \tag{12}$$

Fluorescence yield for the band system

$$\varepsilon^{system} = N \frac{\sigma_{00}^{eff}(E,P)}{q_{X \to 0}\, B^{00}} \sum_{vv'} q_{X \to v} B^{vv'} \frac{P'_v}{P + P'_v} \tag{13}$$

1N molecular parameters

v/ v'	0	1	2	3	5	5	$q_{X\rightarrow v}$	P^{v}_{nitr} (hPa)	P^{v}_{air} (hPa)
0	391.2 0.627	427.5 0.204	470.6 0.043	522.5 0.007	586.1 0.001	665.9 0.000	0.883	1.7	1.3
1	358.0 0.041	388.2 0.029	423.4 0.030	464.9 0.011	514.6 0.003	575.0 0.001	0.114	–	–
2	330.5 0.000	356.1 0.001	385.5 0.000	419.7 0.000	459.7 0.000	570.4 0.000	0.002	–	–

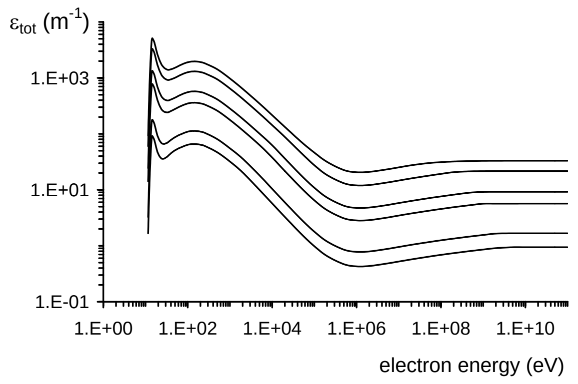
Table 2.- Wavelength (nm) of the v-v' transition (upper number) and product $B^{vv'} \cdot q_{X\rightarrow v}$ (lower number). The horizontal sum of these products is equal to the $q_{X\rightarrow v}$ Franck-Condon factor for the molecular excitation. Characteristic pressures are shown in last rows.

2P molecular parameters

v/ v'	0	1	2	3	4	5	6	7	$q_{X\longrightarrow v}$	P^v_{nitr} (hPa)	P^v_{air} (hPa)
0	337.0 0.265	357.6 0.175	380.4 0.072	405.8 0.022	434.3 0.006	466.5 0.001	503.2 0.000	545.2 0.000	0.545	77	13.1
1	315.8 0.138	333.8 0.007	353.6 0.064	375.4 0.057	399.7 0.028	426.8 0.010	457.3 0.003	491.7 0.001	0.308	36	11.2
2	297.6 0.016	313.5 0.041	330.9 0.003	349.9 0.007	370.9 0.016	394.2 0.013	420.0 0.006	448.9 0.002	0.106	23	9.1
3	281.8 0.001	296.2 0.009	311.5 0.007	328.4 0.003	346.8 0.000	367.1 0.003	389.4 0.004	414.0 0.002	0.030	22	7.9
4	268.4 0.000	281.2 0.000	295.2 0.003	310.2 0.001	326.6 0.001	344.5 0.000	364.1 0.000	385.6 0.001	0.008	21	6.7

Table 3.- Same as table 2 for the 2P system

Total fluorescence yield (300 - 406 nm) for pure nitrogen



Pressures (bottom - up) 1, 2, 10, 20, 100 and 1013 hPa

Fluorescence yield at high pressure and high energy

High pressure

$$\varepsilon_{vv'} \sim q_{X\to v} B^{vv'} P'_v \text{ (relative intensities)} \tag{14}$$

$$\varepsilon^{system} = \frac{1}{kT} \frac{\sigma_{00}^{eff}(E,P)}{q_{X\to 0} B^{00}} \sum_v q_{X\to v} P'_v \,, \tag{15}$$

$E > 10^3$ eV, $P \times R > 3\text{hPa}\times\text{cm}$

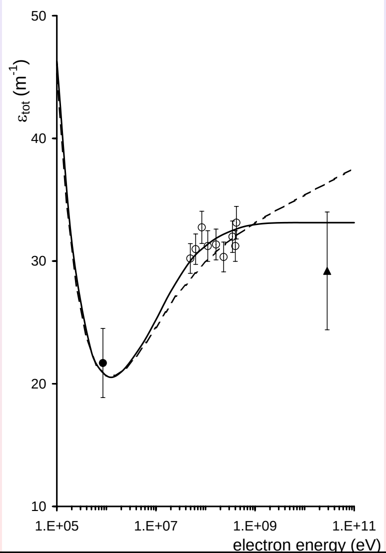
$$\sigma_{00}^{1N,eff}(E,P) = (\chi_{00} + \alpha_{00}^{1N}) \sigma_{ion} \tag{16}$$

$$\sigma_{00}^{2P,eff}(E,P) \approx \alpha_{00}^{2P} \sigma_{ion} \tag{17}$$

$E > 1.3\times10^5$ eV and atmospheric pressure → α = constant

$$\varepsilon \propto \sigma_{ion} \tag{18}$$

Total fluorescence yield (300 - 406 nm) for N_2



Atmospheric pressure

— our calculations

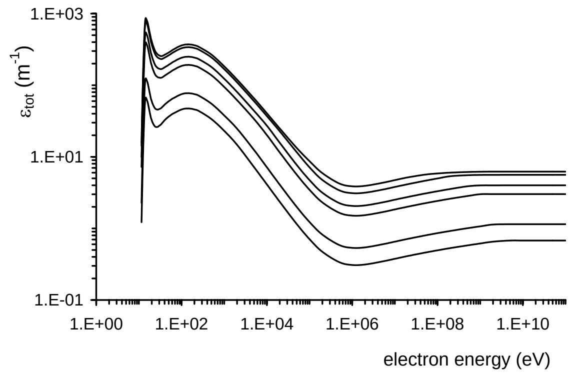
● Nagano et al.

▲ FLASH

○ AIRFLY (normalized)

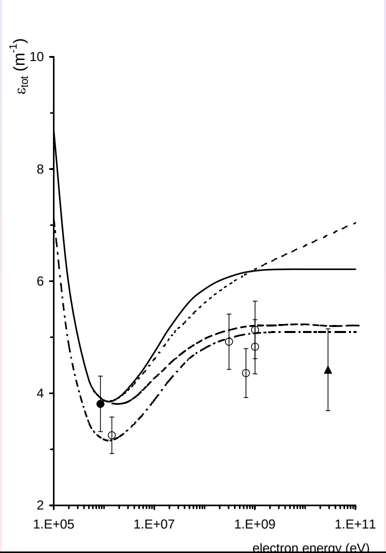
- - - Bethe-Bloch (normalized)

Total fluorescence yield (300 - 406 nm) for dry air



Pressures (bottom - up) 1, 2, 10, 20, 100 and 1013 hPa

Total fluorescence yield (300 - 406 nm) for dry air



Atmospheric pressure

— our calculations

-.-. our calculations ↓ 18%

● Nagano et al.

▲ FLASH

○ Kakimoto et al.

.... Bethe-Bloch (normalized)

- - - normal. deposited energy (FLASH)

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Stopping cross section (Bethe-Bloch)

Electron stopping power $S = \frac{dw}{dx}$, i.e. the energy loss per unit length of traversed matter due to both excitation and ionization processes, can be expressed by

$$S = N \sum E_n \sigma_n = NR_y \sum (E_n/R_y) \sigma_n = NR_y \sigma_{st} \,, \tag{19}$$

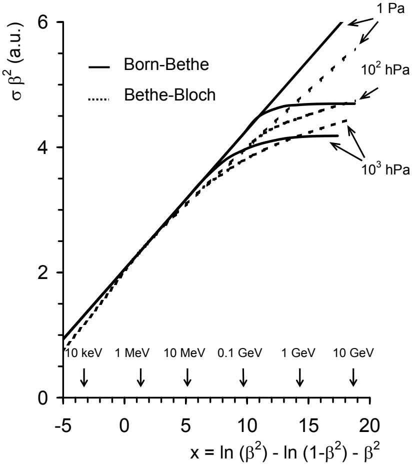
where the *stopping cross section* is defined as

$$\sigma_{st} = \sum (E_n/R_y) \sigma_n \tag{20}$$

E_n is the excitation energy plus the energy transferred to the secondary electron in ionizations.

σ_n is the cross section for the process n (i.e. excitation of the upper level of the 1N and 2P systems are only two of the many, many, many,.. processes involved in the energy loss).

Stopping cross sections and ionization cross section



—— Ionization cross section

- - - Stopping cross section

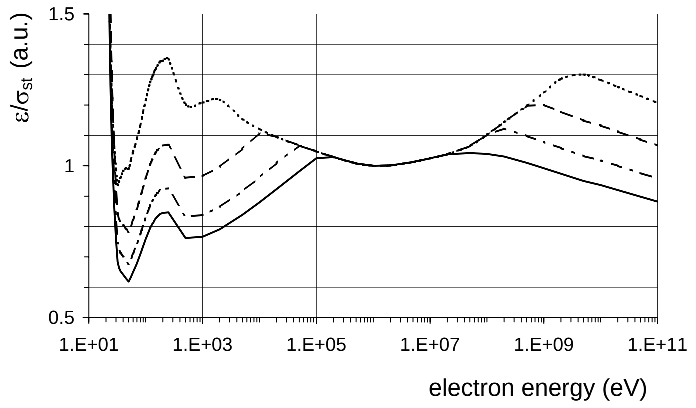
Deposited energy and stopping power

Slow electrons: All the energy is locally deposited ⇒ Deposited energy is given by the stoping power $\sigma_{st}(E)$

Fast electrons: A significant fraction of the energy loss is NOT locally deposited (high energy secondary electrons) ⇒ Deposited energy smaller than expected from $\sigma_{st}(E)$.

Electron energy $\longleftrightarrow$ electron range (E) $\longleftrightarrow$ Region size R $\longleftrightarrow$ local

Fluorescence yield versus stopping power



Pressures (bottom up) 1013 200 20 1 hPa

Fluorescence yield and deposited energy

- The energy spectrum of secondary electrons depends on the primary energy (e.g. increasing primary energy gives rise to higher energy secondaries)
- Fluorescence light is generated by secondary electrons for which ε and σ_{st} (and therefore deposited energy) follow a different E behavior

Therefore

Fluorescence yield is not expected to be (exactly) proportional to deposited energy.

Conclusions

- A general procedure for the calculation of fluorescence yield in a very wide energy interval ranging from threshold up to the GeV region is shown.
- Particular attention has been paid to the the contribution of secondary electrons ejected in ionization processes.
- Comparison of our predictions with available measurements at high energy ($E > 1$MeV) and high pressure shows very good agreement for pure nitrogen while some discrepancies of about 20% are found for dry air. These discrepancies are very likely due to uncertainties in the quenching cross sections.
- Fluorescence yield is not expected to be proportional to deposited energy. A comparison of our fluorescence yield results with deposited energy in the FLASH experiment shows a deviation from proportionality of about 20% in the interval 1 MeV - 10 GeV.

more details in:

F. Arqueros et al., submitted to Astroparticle Physics and available in arXiv:astro-ph/0604498 v1 24 Apr 2006