Nitrogen fluorescence yield in dependence on atmospheric conditions

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The effective fluorescence yield in air is a crucial quantity for the reconstruction of extensive air showers detected with fluorescence telescopes. Several laboratory experiments provide results for the fluorescence yield that is typically measured in small scintillation chambers. These data are compared to a theoretical description of the dependence on atmospheric conditions.

1. Introduction

In several air shower experiments (e.g. HiRes, Pierre Auger Observatory, TA [1]), the fluorescence technique for detecting extensive air showers is employed. Measuring the fluorescence light that nitrogen molecules emit after being excited by charged particles traversing the atmosphere, is the most direct method of detecting the longitudinal shower profile. For the reconstruction procedures of the air shower experiments, the value of fluorescence yield FY_{λ} and its dependence on atmospheric conditions are crucial parameters.

The theory of fluorescence light emission is based on the *Franck-Condon principle* and the theory of molecular motion. The absolute value of FY_{λ} is measured by different laboratory experiments. In this article, we want to compare results of different laboratory measurements with theoretical calculations, accounting for the atmospheric conditions.

2. Theoretical description of fluorescence emission and comparison of measurements

The N₂ fluorescence spectrum is characterized by an electronic band system. Light is emitted isotropically mainly in the wavelength region between 300 and 400 nm. Up to now, there are 19 strong emission bands separated, 18 of them are belonging to the second positive (2P) system and the other to the first negative system (1N). Nitrogen molecules are excited mainly by electrons which are most numerous charged particles in extensive air showers. During de-excitation some non-radiative processes have to be taken into account. Therefore, the quantum efficiency of fluorescence is defined as

$$\frac{\text{rate of de-excitation via radiation}}{\text{total rate of de-excitation}} = \frac{\tau_c}{\tau_0 + \tau_c},$$
(1)

where the rate of de-excitation is proportional to the reciprocal of the life time. The mean life time of a radiative transition to any lower state is τ_0 , and to collisional quenching τ_c . The collisional quenching depends on the collision rate and, therefore, on the mean velocity of molecules $\overline{v} = \sqrt{\frac{8kT}{\pi M}}$:

$$\tau_c = (\sqrt{2} \cdot \rho_n \cdot \sigma_{\rm NN} \cdot \overline{v})^{-1} = \sqrt{(\pi M/kT)} \cdot (4\rho_n \cdot \sigma_{\rm NN})^{-1},$$
(2)

where ρ_n is the particle number density, σ_{NN} the collisional cross section between nitrogen molecules, T the temperature, k the Boltzmann constant, and M the molecular mass. Now the fluorescence efficiency can be defined as

$$\varepsilon_{\lambda}(p,T) = \frac{\varepsilon_{\lambda}(p \to 0)}{1 + (p/p'_{\nu}(T))} = \frac{\text{radiated energy in the form of fluorescence photons}}{\text{energy deposit in the observed medium}} = \frac{n \cdot E_{\gamma}}{E_{dep}}, \quad (3)$$

with $\varepsilon_{\lambda}(p \to 0)$ being fluorescence efficiency at wavelength λ without collisional quenching, *n* denoting the number of photons, and $p/p'_{\nu} = \tau_{0,\nu}/\tau_{c,\nu}$. The pressure *p* is that of the observed medium (e.g. air), p'_{ν} is a

reference pressure, $\tau_{0,\nu}$, and $\tau_{c,\nu}$ are the mean life times for excitation level ν . Applying actual atmospheric conditions, with air presumed to be a two-component gas, the relation between p and p' can be written as

$$\frac{p}{p_{\nu}'} = \tau_{0,\nu} \cdot \left(\frac{1}{\tau_{\mathrm{NN},\nu}(\sigma_{\mathrm{NN},\nu})} + \frac{1}{\tau_{\mathrm{NO},\nu}(\sigma_{\mathrm{NO},\nu})}\right) = \frac{\tau_{0,\nu} p_{\mathrm{air}} \cdot N_A}{R \cdot T} \cdot \sqrt{\frac{kTN_A}{\pi}} \cdot \left(4 \cdot vol\%(\mathrm{N}_2) \cdot \sigma_{\mathrm{NN},\nu} \sqrt{\frac{1}{\mathrm{M}_{\mathrm{m},\mathrm{N}}}} + 2 \cdot vol\%(\mathrm{O}_2) \cdot \sigma_{\mathrm{NO},\nu} \sqrt{2(\frac{1}{\mathrm{M}_{\mathrm{m},\mathrm{N}}} + \frac{1}{\mathrm{M}_{\mathrm{m},\mathrm{O}}})}\right),$$
(4)

with Avogadro's number N_A , the masses per mole for nitrogen $M_{m,N}$ and oxygen $M_{m,O}$, and the cross sections for collisional de-excitation for nitrogen-nitrogen $\sigma_{NN,\nu}$ and nitrogen-oxygen $\sigma_{NO,\nu}$.

The here shown calculations are based on theoretical expectations and some free parameters which have been obtained by fluorescence measurements. Values for $\varepsilon_{\lambda}(p \to 0)$, see table 2, are given in [2] and also the deactivation constants, see Table 1, are taken from [2] or partly exchanged by recent data from [3].

		Bunner [2]		Ulrich et al. [3]			
	$\sigma_{ m NO} \ { m in m}^2$	${m \sigma}_{m Nm N}$ in m 2	$ au_{0}$ in 10^{-8} s	${m \sigma}_{m Nm N}$ in m 2	$\sigma_{ m Nvapor} \ { m in} \ { m m}^2$	$ au_0$ in 10 ⁻⁸ s	
$1N \nu = 0$	13×10^{-19}	4.37×10^{-19}	6.58	-	-	-	
$2P \nu = 0$	2.1×10^{-19}	1.0×10^{-20}	4.45	1.82×10^{-20}	8.53×10^{-19}	4.17	
$\nu = 1$	$5.0 \times 10^{-19} a$	3.5×10^{-20}	4.93	3.77×10^{-20}	8.04×10^{-19}	4.17	
$\nu = 2$	$7.0 \times 10^{-19} a$	8.8×10^{-20}	4.45	-	-	-	
$\nu = 3$	$8.0 \times 10^{-19} a$	1.2×10^{-19}	6.65	-	-	-	

Table 1. Deactivation constants for air in the lower atmosphere

^a This value is determined by the given results of [2] and not given in his original publication.

Wavelength-dependent results of fluorescence yield measurements have been provided by 3 experiments [2, 4, 5]. Bunner lists several intermediate values: $\varepsilon_{\lambda}(p \to 0)$, $\varepsilon_{\lambda}^{s.l.}(p,T)$ in %, and the fluorescence efficiency $\varepsilon_{E_{dep}}^{s.l.}$ in units of photons/MeV of deposited energy = $\varepsilon_{\lambda}^{s.l.}(p,T) \cdot (\lambda/hc)$, with λ = wavelength, c = speed of light, h = Planck's constant, at sea level (s.l.). The values for $\varepsilon_{\lambda}^{s.l.}(p,T)$ and $\varepsilon_{E_{dep}}^{s.l.}$ given explicitly in [2] are not reproduced by the here shown calculations, see Table 2. Possible reasons are rounding uncertainties by Bunner or the use of deviating numbers for variables concerning air conditions. Davidson and O'Neil list results for $\varepsilon_{\lambda}^{s.l.}(p,T)$ for wavelengths above 328 nm [4]. It should be mentioned that the results in [4] are given for p = 800 hPa. However, the pressure dependence is not so strong in this region from sea level with p = 1013 hPa to p = 800 hPa. Nagano et al. report directly the values for FY_{λ} at sea level for 0.85 MeV electrons [5], however, only 10 contributing emission bands are listed. For comparing the results of all authors, 0.85 MeV electrons are chosen as exciting particles, so the ionization energy deposit is dE/dX = 0.1677 MeV/kg·m⁻² [6]. It is assumed that the fluorescence yield is proportional to the energy deposit as indicated by experiments [7, 8]. Air is taken to be a composition of 78.8 % N₂ and 21.1 % O₂ [6]. The resulting fluorescence yield can be written as

$$FY_{\lambda} = \varepsilon_{\lambda}(p,T) \cdot \frac{\lambda}{hc} \cdot \frac{dE}{dX} \cdot \rho_{air} \left[\frac{\text{photons}}{\text{m}}\right].$$
(5)

A comparison of the obtained FY_{λ} values at sea level is shown in Table 2.

Kakimoto et al. provide a formula for calculating the fluorescence yield between 300 and 400 nm, which gives at sea level 3.275 $\frac{\text{photons}}{\text{m}}$ [7]. This value is smaller by 11 % compared to the results of Nagano et al. The HiRes

			Fluorescence Yield $FY_{\lambda}^{s.l.}$						
Wave-		$arepsilon_\lambda$	Bunner	Davidson &	this work with	this work with	Nagano		
length	Band	$(p \rightarrow 0)$	[2]	O'Neil [4]	Tab. 1 _{Bunner}	Tab. 1_{Ulrich}	et al. [5]		
λ (nm)		(%)	$\left(\frac{\text{photons}}{\text{m}}\right)$	$\left(\frac{\text{photons}}{\text{m}}\right)$	$\left(\frac{\text{photons}}{\text{m}}\right)$	$\left(\frac{\text{photons}}{\text{m}}\right)$	$\left(\frac{\text{photons}}{\text{m}}\right)$		
311.7	2P (3-2)	.005	0.008	-	0.009	0.009	_a		
313.6	2P (2-1)	.029	0.090	-	0.094	0.094	_a		
315.9	2P (1-0)	.050	0.224	-	0.240	0.279	0.549		
328.5	2P (3-3)	.0154	0.027	0.035	0.029	0.029	0.180		
330.9	2P (2-2)	.002	0.007	_a	0.007	0.007	_a		
333.9	2P (1-1)	.0041	0.019	_a	0.021	0.024	_a		
337.1	2P (0-0)	.082	0.887	1.173	1.169	1.109	1.021		
346.9	2P (3-4)	.0063	0.012	0.015	0.013	0.013	_ ^a		
$350.0(1)^{b}$	2P (2-3)	.004	0.014	0.013	0.014	0.014	_a		
353.7	2P (1-2)	.029	0.146	0.188	0.156	0.181	0.130		
357.7	2P (0-1)	.0615	0.707	0.889	0.930	0.882	0.799		
367.2	2P (3-5)	.0046	0.009	0.012	0.010	0.010	_a		
371.1	2P (2-4)	.010	0.037	0.047	0.038	0.038	_a		
375.6	2P (1-3)	.0271	0.150	0.187	0.155	0.180	0.238		
380.5	2P (0-2)	.0213	0.261	0.328	0.343	0.325	0.287		
389.4	2P (3-6)	.003	0.006	_a	0.007	0.007	_a		
391.4	1N (0-0)	.33	0.281	0.454	0.315	0.315	0.302		
394.3	2P (2-5)	.0064	0.025	0.032	0.026	0.026	0.063		
399.8	2P (1-4)	.016	0.090	0.119	0.097	0.113	0.129		
sum of $\lambda = (300 - 400)$ nm			3.001	3.490 ^c	3.672	3.653	3.698		
sum of all Nagano-wavelengths			2.798	3.404 ^c	3.460	3.438	3.698		

Table 2. Fluorescence yields at sea level in the US Std. Atmosphere. Details see text.

^a This transition has not been measured.

^b In the work of Davidson & O'Neil, the wavelength for this transition is given with 350.1 nm.

^cOnly measurements above 328 nm.

Collaboration uses a value of about 5 $\frac{\text{photons}}{\text{m}}$ per charged particle in an air shower [9]. For these charged particles, an average energy deposit of 0.22 MeV/kg m⁻² is assumed [2], which leads to a corresponding fluorescence yield at s.l. of 3.811 $\frac{\text{photons}}{\text{m}}$ for a 0.85 MeV electron. Assuming that the HiRes value refers to 5 km a a lagram would abte in the lagram of a 2.2 mbatons. The second se 5 km a.s.l., one would obtain at s.l. 3.6 - 3.7 $\frac{\text{photons}}{\text{m}}$. The calculations shown here reproduce the measured values from Nagano very accurately and the partly varying deactivation constants do not affect the final result much. However, this holds only for the comparison of the whole wavelength region between 300 and 400 nm. One difficulty in these measurements is the treatment of interference filter which have a bandwidth of about 10 nm [5]. The 10 contributions of Nagano et al. are given after subtracting additional contributions by smaller emissions. Thus, for a direct comparison, one has to take into account only the 10 wavelengths reported in [5] and in this case, the calculations differ by approximately -7%.

Altitude dependence of the fluorescence yield 3.

The formulas given in Sec. 2, provide directly the fluorescence yield in dependence on pressure and temperature. Other authors deduce parameterizations of functional forms based on the same equations [5, 7]:

$$FY_{\lambda}^{[5]} = \frac{dE}{dX} \cdot \left(\frac{A_{\lambda}\rho}{1+\rho B_{\lambda}\sqrt{T}}\right), \qquad FY_{300-400\ nm}^{[7]} = \frac{dE}{dX} \cdot \rho \left(\frac{A_{1}}{1+\rho B_{1}\sqrt{T}} + \frac{A_{2}}{1+\rho B_{2}\sqrt{T}}\right). \tag{6}$$

Both types of ansätze predict similar height dependence, see Fig. 1. The parameterization differs from the direct calculation by less than 1.5 %. In Fig. 2, the variation of the altitude dependence due to seasonal effects is illustrated. The two exemplarily chosen atmospheres are representatives for conditions in Argentina at the southern site of the Pierre Auger Observatory [10]. The relative difference to the US Std. Atmosphere is shown in Fig. 3. During winter, the variation is smallest and below 1.5 %. However during summer, the difference is about -2.5 to -3 % in the altitude range most important for air shower detection.



Figure 1. FY in dependence on altitude in the US Std. Atmosphere.





Figure 2. Fluorescence yield as function of altitude in three different atmospheres as given in [10].

Figure 3. Difference in *FY* of two representative Argentine atmospheres to the US Std. Atmosphere.

For the 337.1 nm emission band, the effect of quenching due to water vapor has been studied. Applying the constants from Tab. 1 by Ulrich et al. and assuming 100 % rel. humidity, the emission at sea level is reduced by ≈ 20 %, at 4 km a.s.l. by ≈ 5 %, and at 8 km a.s.l. just by 0.3 %.

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