



## Chromographs Limited Rotational Diffusion and Their Importance in the Calculation of Correlation Functions

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**Abstract:** This article describes the measurement of translational and rotational diffusion coefficients by light scattering techniques and discusses several applications of these techniques to studies in enzymology, including molecular weight determination, absolute size and shape of enzymes in solution, and observation of conformational changes during protein denaturation. The chapter also describes the problems of sample polydispersity and multiple scattering. Light-scattering techniques have long provided powerful methods for the determination of macromolecular weight, size, and shape. These studies rely upon the accurate determination of the intensity of the light scattered by solutions of macromolecules. Because the lifetimes of the random fluctuations in dielectric constant that produce this scattering are so long compared with the period of the incident light, the spectrum of the scattered light is far too narrow to have been measured before the recent advent of laser light sources, light-mixing spectroscopic techniques.

**Keywords:** rotational diffusion, molecule, atom,

### INTRODUCTION

The corrected rotational diffusion coefficient for a rod in the free molecular regime is given in this work and a simplified derivation using the differential drag forces for a rotating rod in the free molecular regime is presented.

Calculations based on the theory of molecular scattering and absorption of light from substances consisting of multi-atomic complex molecules should take into account the internal movement of molecules, including limited rotational movement. Because, in some cases, such a movement can cause a change in the induced dipole moment or polarization tensor. In turn, this scattering or absorption causes a change in intensity.

1. It is known that the intensity of infrared absorption

$$I(\omega) = A \int (\mu_x(0) \mu_x(t)) \exp(-i\omega t) dt$$

2. Rayleigh scattering of light

$$I(\omega) = \int (a(0) d(t)) e^{-i\omega t} dt$$

Rayleigh scattering results from the electric polarizability of the particles. The oscillating electric field of a light wave acts on the charges within a particle, causing them to move at the same frequency. The particle, therefore, becomes a small radiating dipole whose

radiation we see as scattered light. The particles may be individual atoms or molecules; it can occur when light travels through transparent solids and liquids, but is most prominently seen in gases.

Rayleigh scattering of sunlight in Earth's atmosphere causes diffuse sky radiation, which is the reason for the blue color of the daytime and twilight sky, as well as the yellowish to reddish hue of the low Sun. Sunlight is also subject to Raman scattering, which changes the rotational state of the molecules and gives rise to polarization effects.[2]

Rayleigh scattering causes clouds to appear colored. In this picture, it is due to the Tyndall effect that scatters the light on smoke particles during the 2021 Mexico forest fire season.

Scattering by particles with a size comparable to or larger than the wavelength of the light is typically treated by the Mie theory, the discrete dipole approximation and other computational techniques. Rayleigh scattering applies to particles that are small with respect to wavelengths of light, and that are optically "soft" (i.e., with a refractive index close to 1). Anomalous diffraction theory applies to optically soft but larger particles.

When calculated using the second formula, the expressions in this represent the correlation function. Therefore, to calculate the absorption or scattering spectra, it is necessary to calculate the correlation functions of the relevant quantities. The following model is used to account for limited circular diffusion. We assume that the orientation of the linear fragment of the molecule is defined by the unit vector  $\vec{u}$ . It is oriented along the linear fragment axis and has spherical polar coordinates  $\Omega = (\theta, \Phi)$ . A linear fragment of a molecule can freely diffuse within an empty cone with a maximum polar angle  $\theta = \theta_0$ , and the axis of the cone passes along the z axis. This model is called the restricted diffusion model. In this model, the polar angle is constrained  $0 \leq \theta \leq \theta_0$  but the azimuthal angle is not constrained.

The finite rotational diffusion model  $\vec{u}(\theta, \varphi)$  unit vector rotates inside a cone with spherical angle  $\theta$ .

At the moment of time t, the probability density of observation of the orientation  $s(\vec{u}, t)$ , i.e. rotation  $s(\vec{u}, t)$  satisfies the rotation diffusion equation.

$$\frac{\partial c(\vec{u}, t)}{\partial t} = D_R \frac{1}{\sin^2 \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{\partial^2}{\partial \Phi^2} \right) c_{\vec{u}, t}$$

Here  $D_R$  is the rotational diffusion coefficient

A technique for the spectroscopic detection of pure rotator Brownian movement of anisotropic macromolecules in solution are developed in combination with a high-resolution optical heterodyne spectrometer. The line broadening originating in the translational diffusion of the solute macromolecule, which is a dominant factor in intensity in the Rayleigh component, is suppressed by taking the forward scattering. Then, only the depolarized light whose amplitude is fully modulated by the rotation of solute molecules is filtered off by the polarizer and received by a photomultiplier tube. The time-dependent component of the output from the phototube is analyzed by a wave analyzer to give a spectrum of the scattered light.

The mean squared displacement in time  $\Delta t$  of a particle undergoing Brownian motion (translational diffusion) in  $d$  dimensions is  $\langle x^2 \rangle = 2dD\Delta t$ , where the diffusion coefficient  $D = \frac{k_B T}{6\pi\eta r}$ , where " $\eta$ " is the dynamic viscosity, " $r$ " is the radius of the spherical particle, " $k_B$ " is Boltzmann's constant and " $T$ " is the absolute temperature.

Similarly, the mean-square angular deviation for rotational diffusion is given by  $\langle \theta^2 \rangle = 2Dr\Delta t$ , where the rotational diffusion coefficient  $D_r = \frac{k_B T}{8\pi\eta r^3}$ .

Equipped with this, it is clear that there are many common factors that cancel when dividing one by the other, leading to

$$\frac{\langle x^2 \rangle}{\langle \theta^2 \rangle} = \frac{4d^3 r^2}{4d^3 r^2},$$

which for example, "in three dimensions, a spherical particle on average rotates by about 1 rad in the time it is displaced by the distance equal to its diameter".

### Conclusion

Polarized dynamic light scattering (DLS) gives access to orientation-averaged translational and rotational diffusion coefficients of anisotropic particles dispersed in fluids in a single experiment. As the combination of both diffusivities contains information on the morphology of the particles, their simultaneous and accurate measurement for the same sample and thermodynamic state is beneficial for particle characterization.

### Literature

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