Förster-resonance-energy transfer FRET

Also contains definition of: dipole-dipole excitation transfer

Non-radiative excitation transfer between two molecular entities separated by distances considerably exceeding the sum of their van der Waals radii. It describes the transfer in terms of the interaction between the transition (dipole) moments of the entities in the very weak dipole-dipole coupling limit. It is a Coulombic interaction frequently called a dipole-dipole coupling. The transfer rate constant from donor to acceptor, $k_{\rm T}$, is given by

$$k_{\rm T} = k_{\rm D} \left(\frac{R_0}{r}\right)^6 = \frac{1}{\tau_{\rm D}^0} \left(\frac{R_0}{r}\right)^6$$

where $k_{\rm D}$ and $\tau_{\rm D}^0$ are the emission rate constant and the lifetime of the excited donor in the absence of transfer, respectively, *r* is the distance between the donor and the acceptor and R_0 is the critical quenching radius or Förster radius, i.e., the distance at which transfer and spontaneous decay of the excited donor are equally probable $(k_{\rm T} = k_{\rm D})$ (see Note 3).

 R_0 is given by

$$R_0 = Const. \left(\frac{\kappa^2 \Phi_D^0 J}{n^4}\right)^{1/6}$$

where κ is the orientation factor, Φ_D^0 is the fluorescence quantum yield of the donor in the absence of transfer, *n* is the average refractive index of the medium in the wavelength range where spectral overlap is significant, *J* is the spectral overlap integral reflecting the degree of overlap of the donor emission spectrum with the acceptor absorption spectrum and given by

$$J = \int_{\lambda} I_{\lambda}^{\rm D}(\lambda) \, \varepsilon_{\rm A}(\lambda) \, \lambda^4 {\rm d}\lambda$$

where $I_{\lambda}^{\rm D}(\lambda)$ is the normalized spectral radiant intensity of the donor so that $\int I_{\lambda}^{\rm D}(\lambda) d\lambda = 1$. $\varepsilon_{\rm A}(\lambda)$ is the molar decadic absorption coefficient of the acceptor. See

Note 3 for the value of *Const.*. Notes:

^{1.} The bandpass $\Delta \lambda$ is a constant in spectrophotometers and spectrofluorometers <u>using gratings. Thus, the scale is linear in wavelength and it is convenient to express</u> IUPAC Compendium of Chemical Terminology Copyright © 2014 IUPAC

and calculate the integrals in wavelengths instead of wavenumbers in order to avoid confusion.

2. In practical terms, the integral $\int_{\lambda} I_{\lambda}^{D}(\lambda) d\lambda$ is the area under the plot of the donor

emission intensity versus the emission wavelength.

3. A practical expression for R_0 is:

$$\frac{R_0}{\mathrm{nm}} = 2.108 \times 10^{-2} \left\{ \kappa^2 \, \Phi_\mathrm{D}^0 \, n^{-4} \, \int_{\lambda} I_{\lambda}^\mathrm{D}(\lambda) \left[\frac{\varepsilon_\mathrm{A}(\lambda)}{\mathrm{dm}^3 \, \mathrm{mol}^{-1} \, \mathrm{cm}^{-1}} \right] \left(\frac{\lambda}{\mathrm{nm}} \right)^4 \mathrm{d}\lambda \right\}^{1/6}$$

The orientation factor κ is given by

$$\kappa = \cos\theta_{\rm DA} - 3\cos\theta_{\rm D}\cos\theta_{\rm A} = \sin\theta_{\rm D}\sin\theta_{\rm A}\cos\varphi - 2\cos\theta_{\rm D}\cos\theta_{\rm A}$$

where θ_{DA} is the angle between the donor and acceptor moments, and θ_D and θ_A are the angles between these, respectively, and the separation vector; φ is the angle between the projections of the transition moments on a plane perpendicular to the line through the centres. κ^2 can in principle take values from 0 (perpendicular transition moments) to 4 (collinear transition moments). When the transition moments are parallel and perpendicular to the separation vector, $\kappa^2 = 1$. When they are in line (i.e., their moments are strictly along the separation vector), $\kappa^2 = 4$. For randomly oriented transition (dipole) moments, e.g., in fluid solutions, $\kappa^2 = \frac{2}{3}$.

4. The transfer quantum efficiency is defined as

$$\varPhi_{\rm T} = \frac{k_{\rm T}}{k_{\rm D} + k_{\rm T}}$$

and can be related to the ratio $\frac{r}{R_0}$ as follows:

$$\Phi_{\rm T} = \frac{1}{1 + \left(\frac{r}{R_0}\right)^6}$$

or written in the following form :

$$\Phi_{\rm T} = 1 - \frac{\tau_{\rm D}}{\tau_{\rm D}^0}$$

where $\tau_{\rm D}$ is the donor excited-state lifetime in the presence of acceptor, and $\tau_{\rm D}^0$ in the absence of acceptor.

- 5. FRET is sometimes inappropriately called fluorescence-resonance energy transfer. This is not correct because there is <u>no fluorescence</u> involved in FRET.
- 6. Foerster is an alternative and acceptable spelling for Förster.

Source:

PAC, 2007, 79, 293 (Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)) on page 342