FEATURES OF ELECTRONIC EXCITATIONS SPIN-SELECTIVE ANNIHILATION IN DNA-SOLUTIONS AND PROTEIN STRUCTURES

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In structural systems, such as biopolymer solution, there are specific particularities of the bimolecular reactions kinetic modes. First of all this is connected with the microheterogeneity of these systems, as well as a conformation mobility of macrochains. Some reagents may be connected with the chain track. As a result of conformation transfer the distance between small molecules will change. In his turn the radiationless electronic excitation energy transfer kinetics acquires new peculiarities as well as the spin-selective annihilation of triplet excitations.

Chain fragments conformation oscillations can compare with a 1d motion in potential $V(z)$ like the parabolic type. Moreover it will accepted a suggestion about descending branch with a slope F of this potential in certain point $z=b$. Then there is an outflow of the probability from the potential pit through the potential peak. An existence of such decay channel is very important for the appearance of a magnetic effect: it is non-spin-selective and besides that competitive versus the pair singlet annihilation channel.

Fig. 1.
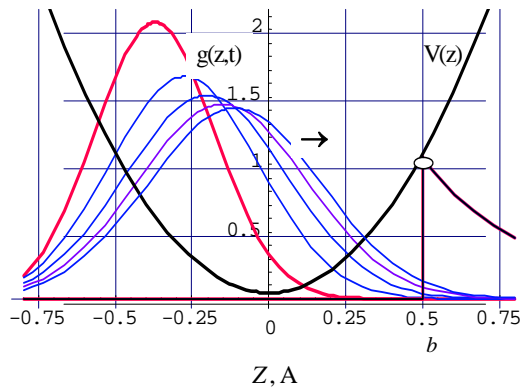
A mathematical model of the process is founded on Fokker-Plank's equation with the broken parabolic potential $V(z) = \kappa z^2 / 2$ (Fig. 1). Its solution has the following form

$$g(z,\xi;t) = \frac{1}{\sqrt{\pi\theta(t)}} \exp\left[-\frac{[z - \xi\exp(-t/\tau_T)]^2}{\theta(t)} \right], \quad (1)$$

where (D – diffusion constant in the field)

$$\theta(t) = 2D\tau_T[1 - \exp(-2t/\tau_T)]; \quad \tau_T = k_B T /(\kappa D).$$

The probability flow from the potential pit with coordinate $z=b$ is given by following

$$j(b,\xi;t) = D\left[\frac{2[b - \xi\exp(-t/\tau_T)]}{\theta(t)} + \frac{F}{k_B T} \right] g(b,\xi;t) ,$$

where the function $g(z,\xi;t)$ is defined by (1). If $t \to \infty$ it is received a stationary density flow

$$j_{stat}(b) = D\left[\frac{b}{D\tau_T} + \frac{F}{k_B T} \right] g_{eq}(b) = D\sqrt{\frac{\kappa}{2\pi k_B T}}\left(\frac{\kappa b + F}{k_B T} \right)\exp\left(-\frac{\kappa b^2}{2k_B T} \right).$$

Function $W(t)$ is the probability of a non-outcome from the potential pit in the time t

$$W(t) = \exp\left[-\int_0^t j(b,\xi; t')dt' \right].$$

The magneto sensitive TT-annihilation rate $K_{ann}(B)$ is given by

$$K_{ann}(B) = K_D\left[\frac{1}{9}\alpha + \left(1 - \frac{1}{9}\alpha\right)\alpha\int_0^\infty \langle 00 | \rho_{T,Q}(t|B) | 00 \rangle \chi(t)W(t)dt \right], \quad (2)$$

where the non spin-selective (spinless) rate

$$\chi(t) = \int_V U(z)g(z,t \mid z',t') \, dz, \qquad (3)$$

$U(z)$ - is the distance dependent rate of the exchange-resonant TT-annihilation act; $g(z,\xi;t)$ - is the transient density probability function (1); $\langle 00 \mid \rho_{T,Q} \mid 00 \rangle$ - is a matrix element of spin-density operator of TT-pair in the collective singlet spin station $\mid 00 \rangle$, indexes T and Q denote initial spin pair stations (triplet and quintuplet).

Other peculiarities of the TT-annihilation kinetics and corresponding magnetic effect of its rate will be appear in polyelectrolyte solutions like DNA-solution. DNA molecule presents itself as a polyanion, so it capable to absorb on itself only small cathion molecules.

Small anion molecules interact with cathionic T-centres moving randomly in the potential field of the polyanion, contraions and ions of a salt. Obviously that particularities of the small anion migration exhibit itself in a photoreaction kinetics in the presence of the external magnetic field.
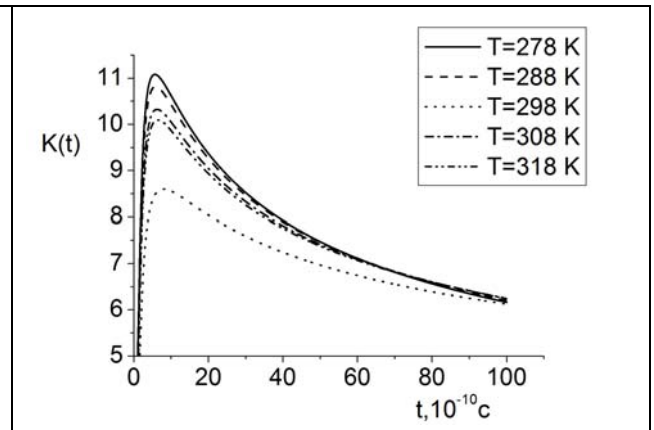
Specific bimolecular reaction rate $K(t)$ is defined as the diffusion flow of small anions to cylindrical surface (around DNA-chain) of radius R

$$K(t) = \frac{4\pi LD}{\Gamma(\beta)} \exp\left[-\frac{U(R)}{kT}\right] \left[\frac{R^2}{4Dt}\right]^{\beta} \exp\left(-\frac{R^2}{4Dt}\right),$$

where $\beta = (kT)^{-1}$, $\Gamma(\beta)$ - gamma-function.
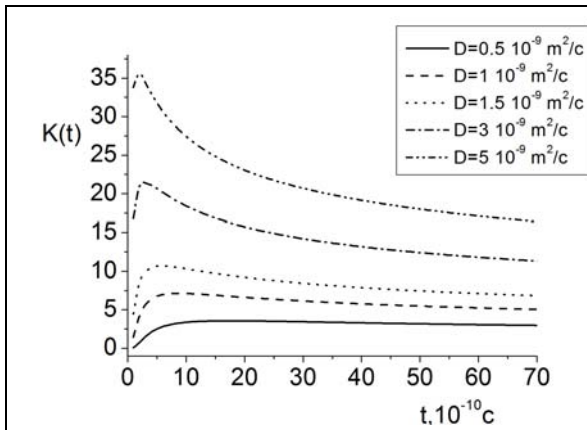
Fig. 2. Time dependence of the bimolecular reaction rate $K(t)$ for different diffusion factors of small molecular anions.

Fig. 3. Time dependence of the bimolecular reaction rate $K(t)$ of small molecules for different temperature of solution.

In applied external magnetic field the formula (2) remains valid still for $K_{ann}(t \mid B)$, but now $W(t) = 1$ and the non spin-selective rate $\chi(t)$ is defined by expression

$$\chi(t) = 2\pi aLD \left[\frac{\partial g}{\partial r} + \frac{1}{kT}\left(\frac{\partial V}{\partial r}\right)g(r,t \mid r')\right]_{r=R},$$

instead of (3).

Coherent TT-pair spin dynamics has relaxation attributes because there is an anion rotational diffusion always. In protein structures with absorbed reagents it has an oscillation nature.