THEORETICAL MODELS OF CHARGE TRANSFER PROCESSES IN NONPOLAR MEDIA

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Abstract: *The charge transfer processes in nonpolar media are considered in the work. The nonpolar medium is regarded as a field of random forces or impulses, and this field acts on the reacting particles. The interaction of reagents with the medium is described through the function of fluctuation of the impulse of a particle of the medium with the speed of the reagent particle. When calculating the kinetic parameters of such a system, the quantum theory of charge transfer processes was used using Green's functions of the impulse density operators of the condensed medium. Analytical expressions for the kinetic parameters of the process are obtained.*
Keywords: *Green's functions, nonpolar medium, multichannel collision theory, charge transfer, quantum theory.*

Introduction

Kinetics of the elementary act of charge transfer processes in nonpolar media

Charge transfer processes in nonpolar media are of great interest of entire fields of knowledge in chemistry, electrochemistry, and photochemistry [1-11]. At the same time, theoretical models for charge transfer processes in polar condensed media have been developed to a much greater extent, see, for example, works [12 - 18].

The transition from polar to non-polar systems by formal extrapolation of the results to low values of dielectric constant at zero frequencies, to low energies of reorganization of the medium, etc. can hardly be considered acceptable. Charge transfer processes in nonpolar media require a completely different approach [19, 20]. One of the approaches of taking into account the non-polar medium in the kinetics of the elementary act of charge transfer processes will be presented in this work.

We will use the multichannel collision theory. We write the complete Hamiltonian of the system in the form:

$$H = H_i + V_i = H_f + V_f \tag{1}$$

Where V_i and V_f are the interactions between reacting particles in the initial and final states, H_i and H_f are the channel Hamiltonians of the initial and final channels.

We write the channel Hamiltonians of the system in the form:

$$H_{i,f} = H_{i,f}^m + H_{i,f}^p + H_{int}^{i,f} \tag{2}$$

Here $H_{i,f}^m$ is Hamiltonian of medium, $H_{i,f}^p$ is the Hamiltonian of reacting particles, $H_{int}^{i,f}$ - is the Hamiltonian of the interaction of particles with the medium, for which we use the following representation:

$$H_{int}^i = - \int \vec{P}(\vec{r})\vec{v}(\vec{r}) \, d\vec{r} \tag{3}$$

Where $\vec{P}(\vec{r})$ - is the fluctuation of impulse at the point $\vec{r}$, $\vec{v}(\vec{r})$ is the speed of the reacting particles.

Interaction in form (3) means that we consider a non-polar medium in the form of a field of random forces or impulses, and this field dynamically affects the reacting particles. Integration is carried out over the entire space over the dimensionless variable $\vec{r}$. If we move from $\vec{r}$ to integration over Cartesian variables, then in formula (3) $\vec{P}$ should be understood as the impulse density.

The probability of an elementary act of charge transfer between particles with the transition of the system from electronic state i to electronic state f has the form:

$$W_{i,f} = \frac{2\pi}{k} \sum_{nn'} e^{\beta(F_i - E_{in})} |\langle \psi_i | V_i | \psi_f \rangle|^2 \, \delta(E_{in} - E_{fn'}) \tag{4}$$

Where ψ_i and ψ_f are the wave functions of the initial and final states of the system, E_{in} and $E_{fn'}$ are the corresponding energy levels, n and n' are all quantum numbers of the system, except electronic ones, F_i is the free energy of the initial state.

Using the integral representation for the δ - function, we reduce formula (4) to the form:

$$W_{i,f} = \frac{\beta}{i} e^{\beta F_i} \int_{-\infty}^{\infty} d\theta Sp[e^{-\beta(1-\theta)H_i} V_i e^{-\beta\theta H_f} V_i] \tag{5}$$

Where the spur (trace) is assumed to be in all coordinates of the system, except electronic ones.

Substituting expressions for channel Hamiltonians (2) into formula (5), we have:

$$W_{i,f} = \frac{\beta}{i} e^{\beta F_i} \int_{-i\infty}^{i\infty} d\theta Sp\left[e^{-\beta(1-\theta)\left[H_i^m + H_i^p + H_{int}^i\right]} V_i e^{-\beta\theta\left[H_f^m + H_f^p + H_{int}^f\right]} V_i\right] \tag{6}$$

We will carry out further calculations in the approximation in which the spur can be divided into two spurs using formula (6) - according to the coordinates of the medium, and according to the coordinates of the reacting particles. This is possible if $\left[H_{i,f}^m + H_{i,f}^p, H_{int}^{i,f}\right] = 0$. If the movement of the reactants is of a classical nature or, in the case of a quantum nature, the changes in the velocities of the reacting particles during the charge transfer process are small, then the commutator can be neglected and for the probability of an elementary act we obtain:

$$W_{i,f} = e^{\beta F_i^m} \int_{-i\infty}^{i\infty} Sp\left[e^{-\beta(1-\theta)\left[H_m + H_{int}^i\right]} e^{-\beta\theta\left[H_m + H_{int}^f\right]} f^p(\theta) d\theta\right] \tag{7}$$

$$f^p(\theta) = e^{\beta F_i^p} Sp\left[e^{-\beta(1-\theta)H_i^p} V_i e^{-\beta\theta H_f^p}\right] \tag{8}$$

Where F_i^m is the free energy of the subsystem $H + H_{int}^i$, F_i^p is the free energy of the reactants in the initial state. When calculating states for non-polar media, the corresponding gas-phase (vacuum) values should be taken as the frequencies of intramolecular vibrations and the equilibrium lengths of the corresponding chemical bonds.

We write V_{if} the electronic resonant integral of the transition of the system from state "i" to state "f" in the form:

$$V_{if} = V_{if}^0 + \Sigma_s b_s Q_s \tag{9}$$

where Q_s are the coordinates of intramolecular vibrations of the reagents.

After calculating the function $f^p(\theta)$ we obtain:

$$f^p(\theta) = e^{\beta F_i^p + \beta\theta(J_i - J_f)} e^{-\beta \Sigma_s E_{rs} \frac{\theta(1-\theta)\omega_s^i \omega_s^f}{(1-\theta)\omega_s^{i\,2} + \theta\left(\omega_s^f\right)^2}} \left[|V_{if}^0|^2 + \Sigma_s\left(V_{if}^0 b_s^* + b_s\right) \frac{\theta\sqrt{2E_{rs}\omega_s^f}\ \omega_s^f}{4\left[(1-\theta)\left(\omega_s^i\right)^2 + \theta\left(\omega_s^f\right)^2\right]} \right] \tag{10}$$

Here J_i and J_f are the minimum energies of impurity in the initial and final states, respectively; F_{ii}^p is the free energy of the reactants in the initial state, E_{rs} is the reorganization energy of the s-th degree of freedom of the regents, ω_s^i, ω_s^f are frequencies of oscillations of the s-th degree of freedom of reagents in the initial and final states, respectively.

Calculation of a spur using the coordinates of the medium can only be carried out approximately. Let's rewrite it in the form:

$$f^m(\theta) = \langle e^{\beta\theta\left(H_m + H_{int}^i\right)} e^{-\beta\theta\left(H_m + H_{int}^i + H_{int}^{fi}\right)} \rangle_i \tag{11}$$

where,

$$H_{int}^{fi} = -\int \vec{P}(\vec{r})\left[\vec{v}^f(\vec{r}) - \vec{v}^i(\vec{r})\right]d\vec{r} \equiv \int d\vec{r}\ \vec{P}(\vec{r})\Delta\vec{v}(\vec{r}) \tag{12}$$

If we introduce the S-matrix for the interaction H_{int}^{fi}, then

$$f^m(\theta) = \langle S(\beta\theta)\rangle \tag{13}$$

where

$$S(\beta\theta) = T_\tau exp\left[-\int_0^{\beta\theta} H_{int}^{fi}(\tau)d\tau\right] \tag{14}$$

Let us expand the exponential in the S-matrix into a series:

$$\langle S(\beta\theta)\rangle_i = \langle T_\tau \sum_{k=0}^{\infty} \frac{1}{k!} \int d\vec{r_1} \int_0^{\beta\theta} d\tau_1 \int d\vec{r_2} \int_0^{\beta\theta} d\tau_2 \ldots \int d\vec{r_k} \int_0^{\beta\theta} d\tau_k\ P_{\alpha_1}(\vec{r_1}\tau_1)$$
$$\times P_{\alpha_2}(\vec{r_2}\tau_2)\ldots P_{\alpha_k}(\vec{r_k}\tau_k)\Delta v_{\alpha_1}(\vec{r_1}\tau_1)\Delta v_{\alpha_2}(\vec{r_2}\tau_2)\ldots\Delta v_{\alpha_k}(\vec{r_k}\tau_k)\rangle_i \tag{15}$$

We will accept the approximation of decoupling quantum statistical averages of fluctuation operators of impulse density into pair averages according to rules similar to those of Wick's theorem [19]. The possibility of carrying out this type of decoupling is described in some detail in [20]. In addition, for $f^p(\theta)$ we will restrict ourselves to the classical approximation. As a result we get:

$$\langle S(\beta\theta)\rangle_i = -\frac{1}{2}\int d\vec{r}\ d\vec{r'} \int_0^{\beta\theta} d\tau_1 \int_0^{\beta\theta} d\tau_2 G_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\tau - \tau'\right)\Delta v_\alpha(\vec{r})\Delta v_\beta\left(\vec{r'}\right) \tag{16}$$

Where $G_{P_\alpha P_\beta}$ is the temperature Green function of the fluctuation operators of the impulse density of the medium:

$$G_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\tau - \tau'\right) = -\langle T_\tau P_\alpha(\vec{r},\tau) P_\beta\left(\vec{r'},\tau'\right)\rangle_i \tag{17}$$

$$A\,\Delta\vec{v}(\vec{r}) = \vec{v}^f(\vec{r}) - \vec{v}^i(\vec{r}) \tag{18}$$

In the Green function $G_{P_\alpha P_\beta}$ we move on to the Fourier representation by τ-τ':

$$G_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\tau - \tau'\right) = -\frac{1}{\beta}\sum_{n=-\infty}^{\infty} G_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\omega_n\right)e^{-i\omega_n(\tau-\tau')} \tag{19}$$

In order to be able to calculate the sum over n and obtain the value of the Green function $G_{P_\alpha P_\beta}$ not only at discrete points ω_n, but also on the entire complex frequency ω plane, it is necessary to move on to the time retarded Green function at finite temperatures $G^R_{P_\alpha P_\beta}$. To do this, we use the correlation relations between the Green functions G_{PP} and G^R_{PP}:

$$G_{PP}(\omega_n) = G^R_{PP}(i\omega_n), \qquad \omega_n > 0 \tag{20}$$
$$G^*_{PP}(\omega_n) = G_{PP}(-\omega_n)$$

and dispersion relations for the Green function G^R_{PP}:

$$G^R_{PP}(\omega_n) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{J_m G^R_{PP}(\omega')}{\omega' - i\omega_n} \tag{21}$$

As a result we get:

$$f^m(\theta) =$$
$$exp\left\{\beta\theta\int d\vec{r}d\vec{r'}\,G^R_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\omega = 0\right)\Delta v_\alpha(\vec{r})\Delta v_\beta(\vec{r}) + \right.$$
$$\left. \frac{1}{\pi}\int_{-\infty}^{\infty} d\vec{r}d\vec{r'}J_m\,G^R_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\omega\right)\Delta v_\alpha(\vec{r})\Delta v_\beta(\vec{r})\frac{sh(\beta\omega(1-\theta)/2\cdot sh(\beta\omega\theta/2)}{sh(\beta\omega/2)}\right\} \tag{22}$$

The Green function of fluctuations of the impulse density of a medium is closely related to all kinds of functions of velocities, forces, and impulses in condensed media. Such correlations make it possible to study the influence of the medium on a specific molecule; obtain an expression for the mean square force acting on the molecule; calculate the diffusion coefficient for the friction coefficient in a liquid; study the processes of thermal conductivity and electrical conductivity (for details on transfer phenomena in condensed systems, see [20]).

Correlation function

The correlation function $K_{\alpha\beta}\left(\vec{r},\vec{r'},\omega\right)$ is the most convenient function for relation with the Green function $G^R_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\omega\right)$. The relationship between these functions has a particularly simple form for the Fourier components:

$$G^R_{P_\alpha P_\beta}\left(\vec{r},\vec{r'},\omega\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{K_{\alpha\beta}\left(\vec{r},\vec{r'},\omega'\right)}{\omega' - \omega - i\delta}, \qquad \delta \to 0 \tag{23}$$

We write the correlation function $K_{\alpha\beta}\left(\vec{r},\vec{r'},\omega\right)$ in the factorization approximation, expressing it through the normalized autocorrelation function of impulses $\Psi(\omega)$ and the correlation function over spatial coordinates $G_{\alpha\beta}\left(\vec{r},\vec{r'}\right)$:

$$K_{\alpha\beta}\left(\vec{r},\vec{r'},t\right) = G_{\alpha\beta}\left(\vec{r},\vec{r'}\right)\Psi(t) \tag{24}$$

For radially symmetric interaction, the function $G_{\alpha\beta}(\vec{r}, \vec{r'})$ can be replaced by the function $\delta_{\alpha\beta} G\left(\left|\vec{r} - \vec{r'}\right|\right)$. As a function $G\left(\left|\vec{r} - \vec{r'}\right|\right)$, you can use a number of model functions of the type:

$$G\left(\left|\vec{r} - \vec{r'}\right|\right) \sim \delta\left(\vec{r} - \vec{r'}\right)$$

$$G\left(\left|\vec{r} - \vec{r'}\right|\right) \sim exp\left[\lambda(\vec{r} - \vec{r'})\right] \tag{25}$$
$$G\left(\left|\vec{r} - \vec{r'}\right|\right) \sim exp\left[\lambda(\vec{r} - \vec{r'})\right] \cdot \cos\left[\mu(\vec{r} - \vec{r'})\right]$$

Where the parameters λ and μ can be defined as fitting ones.

The time dependence of the normalized autocorrelation functions of impulses for various condensed systems has been studied in some detail in a number of works [20]. The most commonly used model of the medium is one in which the motion of atoms is assumed to be oscillations near some average position, which in turn experiences Brownian motion. To describe Brownian motion, the Langevin equation is used for the motion of a molecule in a statistically equilibrium medium.

$$\Psi(\omega) = \frac{2}{\pi} \int_0^\infty \Psi(t) \cos \omega t \, dt, \tag{26}$$

The following expression was obtained in work [20]:

$$\Psi(\omega) = \frac{D}{\pi}\left\{\frac{\gamma^2\gamma'^2}{(\omega^2+\gamma'^2)\omega^2+\gamma^2\gamma'^2} + \frac{\gamma\gamma'}{\omega_0^2}\frac{\lambda\omega^2}{\omega^2+\gamma'^2}\right\} \cdot \left\{\left(\frac{\omega^2-\omega_0^2}{\omega_0^2}\right)^2 + \frac{\omega^2\lambda^2}{\omega^2+\gamma'^2}\right\} \tag{27}$$

Here D is diffusion coefficient in medium, γ is friction coefficient, γ' is characteristic time of decrease of the autocorrelation function of the stochastic force, ω_0 is the cutoff frequency of the spectrum of stochastic forces in the medium, λ is the ratio of the root-mean-square value of the fluctuation of the force acting on the oscillator (an atom performing oscillatory motion) to the root-mean-square value of the fluctuation of the force acting on the center of oscillations and determining the Brownian motion of atoms.

Finally, the velocity for the reactant particles must be determined. The movement of reactants in a field of random forces can be considered in the same way as a condensed nonpolar medium itself is considered.

For reactants, equations for stochastic motion with damping can be written in the form [20]:

$$\frac{d\vec{V}}{dt} + \int_0^t \Gamma(t - t')\vec{V}(t')dt' = \vec{F}(t) \tag{28}$$

This equation is written in matrix form, and here

$$\vec{V}(t) = \begin{bmatrix} d\vec{r}/dt \\ d\vec{R}/dt \end{bmatrix}; \quad \Gamma(t) = \begin{bmatrix} \mu(t) + \omega_0^2 & -\omega_0^2 \\ -\omega_1^2 & \gamma(t) + \omega_1^2 \end{bmatrix}; \quad \vec{F}(t) = \begin{bmatrix} A(t) \\ B(t) \end{bmatrix} \tag{29}$$

Where $\vec{r}$ – describes the instantaneous position of the particle's center of gravity, $\vec{R}$ is the average position of the particle's center of oscillation, $A(t)$ is the fluctuation force in the medium leading to particle oscillations; $B(t)$ is the fluctuation force in the medium, leading to Brownian motion; $\mu(t)$– takes into account the effect of friction force retardation, $\gamma(t)$ is dependence of the friction coefficient on time, ω_1 can be expressed through the corresponding frequency value ω_0: $\omega_1 = \sqrt{\frac{m}{m^*}}\omega_0$, where m is the mass of the particle, m^* is its effective mass (takes into account the mass of the particle and several atoms of the medium surrounding the particle).

Conclusion

The processes of charge transfer in nonpolar media were considered. The nonpolar medium is represented as a field of random forces or impulses, and this field acts on the reacting particles. The interaction of reagents with the environment is represented through the function of fluctuation of the impulses of the particles of the medium with the velocities of the reagent particles.

When calculating the kinetic parameters of such a system, the quantum theory of charge transfer processes was used using Green's functions of the impulse density operators of the condensed medium. Analytical expressions for the kinetic parameters of the process are obtained.

Further calculations require detailing the potentials of intermolecular interactions; the nature of fluctuations of random forces and impulses in the medium; the selection of parameter values from experiments and boundary conditions for solving the given equations.

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QEYRİ-POLYAR MÜHİTDƏ YÜKLƏRİN DAŞINMASI PROSESİNİN NƏZƏRİ MODELLƏRİ

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Xülasə: İşdə qeyri-polyar mühitlərdə yüklərin daşınması prosesləri araşdırılmışdır. Qeyri-polyar mühit kimi təsadüfi qüvvələr və ya impulslar sahəsi hesab olunur və bu sahə qarşılıqlı təsirdə olan hissəciklərə təsir göstərir. Reagentlərin mühitlə qarşılıqlı təsiri mühitdə olan hissəciklərin impulsunun reagentin hissəciklərinin sürətindən asılılıq funksiyası vasitəsilə təsvir edilir. Belə sistemlərin kinetik parametrlərinin hesablanması zamanı kondensə olunmuş mühitin impuls sıxlığı operatorlarının Qrin funksiyalarından və yük daşınması proseslərinin kvant nəzəriyyəsindən istifadə edilmişdir. Prosesin kinetik parametrləri üçün analitik ifadələr alınmışdır.
Açar sözləri: Qrin funksiyaları, qeyri-polyar mühit, çoxkanallı toqquşma nəzəriyyəsi, yük daşınması, kvant nəzəriyyəsi.

ТЕОРЕТИЧЕСКИЕ МОДЕЛИ ПРОЦЕССОВ ПЕРЕНОСА ЗАРЯДА В НЕПОЛЯРНЫХ СРЕДАХ

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Резюме: В работе рассмотрены процессы переноса заряда в неполярных средах. Неполярная среда рассматривается как поле случайных сил или импульсов, и это поле действует на реагирующие частицы. Взаимодействие реагентов со средой описывается через функцию изменения импульса частицы среды со скоростью частицы реагента. При расчете кинетических параметров такой системы использовалась квантовая теория процессов переноса заряда с использованием функций Грина операторов плотности импульса конденсированной среды. Получены аналитические выражения для кинетических параметров процесса.
Ключевые слова: функции Грина, неполярная среда, многоканальная теория столкновений, перенос заряда, квантовая теория.