On the eigenvalues of the operator sum of squares of vector fields

LET Ω be a bounded domain in R^n with smooth boundary and let X_j be a smooth real vector field on $\bar{\Omega}$, $j=1, \cdots, l$. Denote by K the space: $\{u \in L^2(\Omega),\ X_j u \in L^2(\Omega),\ j=1, \cdots, l\}$ with the norm $\| u \|_K = (\| u \|_{L^2}^2 + \sum_{j=1}^{l} \| X_j u \|_{L^2}^2)^{\frac{1}{2}}$ and by K_0 the closure of $C_0^\infty(\Omega)$ in K.

Let $P = -\sum_{j=1}^{l} X_j^2$. We consider the eigenvalue problem:

$$Pu = \lambda u, \quad u \in K_0 \setminus \{0\}. \tag{1}$$

The main results of this letter are the following.

Theorem 1. Suppose that the vector fields X_j $(j=1, \cdots, l)$ satisfy the following conditions:

(i) (Hormander's condition) At each point of $\bar{\Omega}$, the rank of the Lie algebra generated by $\{X_j\}_{j=1}^{l}$ equals n.

(ii) As differential operators, X_j are formally anti-self-adjoint; that is,

$$(X_j u, v) = -(u, X_j v), \text{ for } u, v \in C_0^\infty(\Omega),\ j = 1, \cdots, l.$$

Then the eigenvalues for the eigenvalue problem (1) exist, which are positive and can be arranged in an increasing sequence

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_m \leqslant \lambda_{m+1} \leqslant \cdots$$

such that $\lambda_m \to \infty$ as $m \to \infty$.

Theorem 2. Let Ω be a bounded domain in R^3 with a smooth boundary and let L be an operator

$$L = -(X^2 + Y^2),$$

where $X = \frac{\partial}{\partial x} + 2ky(x^2+y^2)^{k-1}\frac{\partial}{\partial t}$, $Y = \frac{\partial}{\partial y} - 2kx(x^2+y^2)^{k-1}\frac{\partial}{\partial t}$, k being a positive integer. Denote by K_0 the completion of $C_0^\infty(\Omega)$ with the norm $\| u \|_{K_0} = (\| u \|_{L^2}^2 + \| Xu \|_{L^2}^2 + \| Yu \|_{L^2}^2)^{\frac{1}{2}}$. Suppose λ_m to be the mth eigenvalue of the eigenvalue problem

$$Lu = \lambda u, \quad u \in K_0 \setminus \{0\}.$$

Then $\lambda_{m+1} - \lambda_m \leqslant \frac{2}{m}\sum_{j=1}^{m} \lambda_j, \quad m = 1, 2, \cdots.$

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Characterization of microenvironmental polarity of methylated β-cyclodextrin with fluorescent probe method

STUDY of modified cyclodextrin is one of the hot topics in host-guest chemistry recently[1, 2]. In this communication, we used a biological probe, neutral red, to indicate the change of microenvironmental polarity caused by the methylation of the hydroxy existing in the rim of β-cyclodextrin (β-CD) and investigate the photochemical behavior of β-CD before and after modification.

Neutral red (NR) exists in two molecular forms in aqueous solution, namely acidic form and neutral form. In pH 7.2 buffer solution, the neutral form is predominant, which has a fluorescence at 628 nm when excited at 465 nm. The excitation and emission spectra of the neutral form showed a strong dependence on the concentration of β-CD or methylated β-CD (β-MCD). At CD concentration lower than 5×10^{-4} mol/L, the excitation and emission maxima remarkably blue-shifted, however, they slightly blue-shifted when the concentration of CD was higher than 5×10^{-4} mol/L. Under any concentrations of CD, the blue-shift caused by the β-MCD-NR system was higher than that by the β-CD-NR system. It is known that the hypsochromic shift of the excitation and emission wavelengths in aqueous solution indicates a decrease in the polarity of the microenvironment surrounding the fluorophore[3], therefore, it can be concluded that the polarity of the β-MCD cavity is lower than that of the β-CD cavity. This can be explained by assuming the hydrophobicity of the cavity microenvironment is enhanced and the polarity is decreased owing to the modification of methyl group to prevent water molecule from entering the cavity. In pH 5.8 buffer solution, the acidic form is predominant, its maximal excitation and emission wavelengths are 520 and 620 nm, respectively. With the increasing of the concentration of CD, the excitation and emission bands blue-shifted and the fluorescence intensity enhanced. Meanwhile, an interesting dependence of excitation wavelength on the concentration of CD was observed. The excitation band at 520 nm for acidic form gradually decreased whereas the excitation band at 460 nm for neutral form increased with the increasing of CD concentration. This phenomenon appeared earlier in β-MCD-NR system than in β-CD-NR system. When the concentration of β-MCD was larger than 0.000 2 mol/L, an obvious excitation band for neutral form appeared. For β-CD, however, the excitation band for neutral form did not appear clearly until the concentration of β-CD was larger than 0.002 mol/L. Since a high hydrophobic molecule can be more easily included in the CD cavity than a low hydrophobic one, the acidic form of NR may lose a hydrogen ion and form the neutral molecule before entering the CD cavity. Having a lower polarity, β-MCD showed a stronger affinity to neutral molecule than β-CD, resulting in a faster change from the acidic form to the neutral form for NR in β-MCD than in β-CD, and causing a larger hypsochromic shift in the fluorescence spectra of NR regardless of any concentrations of CD. This further confirms that β-MCD has a lower polarity than β-CD.

The effect of alcohol on CD cavity has been generally considered to be the steric hindrance. Alcohol can form hydrogen bond with the primary hydroxy on the rim of small opening of CD cavity, thus the effect of water phase on the cavity of CD is minimized and the polarity of CD cavity is decreased. According to this assumption, it can be expected that the polarity of β-CD cavity should be decreased, thus the molecules of NR should be more easily included into the cavity of β-CD in the presence of methanol. That means the effects of both systems , β-MCD and β-CD with methanol, on NR should be similar. Therefore, for the system of β-CD-NR containing mathanol, the higher the content of methanol, the lower the polarity of β-CD cavity should be, thus the higher the fluorescence intensity of the β-CD-NR system must be. However, the experimental results negated the above expectation. The experimental results showed that with the addition of methanol, the fluorescence intensity of NR decreased, meanwhile, the excitation and emission bonds red-shifted till reaching 510 nm and 613 nm, respectively, which correspond to the excitation and emission maxima of NR, respectively, in methanol medium. The results suggest that the molecules of NR be squeezed out of the cavity of β-CD with the addition of methanol. When the content of methanol was higher than 4%, the excitation and emission peaks were no longer changed, but the fluorescence intensity was enhanced, implying that NR is fully squeezed out of the cavity of β-CD and the effect of methanol on the fluorescence of NR in the β-CD system is similar to that in aqueous solution.

In summary, in acidic or neutral solution, the polarity of β-MCD cavity is smaller than that of β-CD cavity and the pseudo-modification of alcohol to β-CD is completely different from the methylated β-CD.

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