MOLEKULALARNING AYLANMA BRAUN HARAKATIDA DIFFUZIYA TENGLAMASI YECHIMLARINI SFERIK GARMONIKALAR ORQALI KORRELYATSION FUNKSIYASINI IFODALASH

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Annotatsiya. Aylanma Braun harakati modellari ko'pincha suyuqliklardagi molekulyar dinamikani o'rganish uchun dielektrik relaksatsiya, dinamik Kerr effekti, infraqizil yutilish, Ramanning tarqalishi va boshqalar kabi turli zond usullari yordamida olingan spektrlarni tegishli nazariy spektrlar bilan solishtirish uchun ishlatiladi [1-2]. Shu asosda birinchi darajali sferik garmonikalar orqali ayrim tipdagi diffuziya teglamasi yechimlarini korrelyatsion funksiyalarni ifodalashni keltirib chiqaramiz.

Kalit so’zlar: diffuziya, aylanma, dielektrik relaksatsiya, effekt.

Birinchi darajali (ℓ =1) sferik garmonikalar tenglamadan quyidagi natijalarni olish mumkin [3],

$$\langle Y_{1,0}(\Omega(0))\rangle = \langle Y^*_{1,0}(\Omega(t))\rangle = \frac{1}{2}\sqrt{\frac{3}{4\pi}}\left(1+\mu_0\right) \qquad (1)$$

$$\int d\Omega Y^m_{\nu_n^m}(\Omega) = \sqrt{2\pi(1-\mu_0)}\delta_{n1}\delta_{m0} \qquad (2)$$

quyidagini ham hosil qildik.

$$\langle Y_{l,m}(\Omega(0))\rangle = \langle Y^*_{l,m}(\Omega(t))\rangle = \frac{3}{4\pi}\sum_{n=1}^{\infty} D_n^o \exp\left[-\nu_n^o(\nu_n^o+1)D_R t\right] \qquad (3)$$

$$D_n^0 = \frac{(I_n^0)^2}{(1-\mu_0)H_n^0} \qquad (4)$$

$$I_n^0 = \mu_0{}^1 d\mu\mu P^m_{\nu_n^m}(\mu) \qquad (5)$$

$$\langle Y_{1,1}(\Omega(0))Y^*_{1,1}(\Omega(t))\rangle = \frac{3}{8\pi}\sum_{n=1}^{\infty} D_n{}' \exp[-\nu_n^1(\nu_n^1+1)D_R t] \qquad (6)$$

$$D_n{}' = \frac{(J_n^1)^2}{(1-\mu_0)H_n^1} \qquad (7)$$

$$J_b^n = \int_{\mu_0}^{1} d\mu\sqrt{1-\mu^2}P^m_{\nu_n^m}(\mu) \qquad (8)$$

Yuqoridagi olingan natijalardan foydalanib

$$\langle Y_{1,-1}(\Omega(0)Y^*_{1,-1}(\Omega(t))\rangle = \langle Y_{1,1}(\Omega(0))Y^*_{1,1}(\Omega(t))\rangle \qquad (9)$$

Bu korrelyasion funksiyalarning $t=0$ bo'lgandagi qiymatlari sferik garmonikalarning o'rtacha kvadratik muvozanatli qiymatlarini beradi. Bu muvozanatli qiymatlar oson hisoblanadi (3) va (6) tenglamalardagi D_n^0 va D_n^1 koeffisiyentlar uchun «summalar» qoidasini beradi. $t=0$ bo'lgandagi o'rtachalar quyidagicha ifodalanadi.

$$\langle Y_{l,0}(\Omega)Y^*_{k,m}(\Omega)\rangle = \frac{1}{2\pi(1-\mu_0)}\int_0^{2\pi} d\phi \int_{\mu_0 1}^{1} d\mu Y_{l'm'}(\Omega)Y^*_{lm}(\Omega) \qquad (10)$$

Stasionar holat bo'yicha quyidagi o'rtachasi kelib chiqadi

$$\langle Y_{l,0}(\Omega)\rangle = \frac{1}{2}\sqrt{\frac{3}{4\pi}}(1+\mu_0) \qquad (11)$$

bu ifoda (1) - dagi kabi

$$\langle Y_{1,0}(\Omega)Y^*_{1,0}(\Omega)\rangle = \langle Y_{1,-1}(\Omega)Y^*_{1,-1}(\Omega)\rangle = \frac{3}{8\pi}\langle \sin^2\theta\rangle = \frac{1}{8\pi}(2-\mu_0-\mu_0^2) \qquad (12)$$

Agar $m \neq m'$ $\langle Y_{1,m}(\Omega)Y^*_{1,m'}(\Omega)\rangle = 0$, agar $m \neq 0$ $\langle Y_{1,m}(\Omega)\rangle = 0$.

Summalar qoidasi (1) va (6) ifodalarda $t = 0$ qo'yib, ularni (9) va (10) lar bilan taqqoslab topilishi mumkin:

$$\sum_{n=1}^{\infty} D_n^{\,0} = \frac{1}{3}(1+\mu_0+\mu_0^2) \qquad (13)$$

$$\sum_{n=1}^{\infty} D_n^1 = \frac{1}{3}(2-\mu_0-\mu_0^2) \qquad (14)$$

$$\sum_{n=1}^{\infty} (D_n^0 + D_n^1) = 1 \qquad (15)$$

$P^0_{\nu_1^0}(\mu) = 1$ va $H_1^{\,0} = 1-\mu_0$ bo'lgani uchun (5) tenglamadan quyidagi kelib chiqadi:

$$I_1^0 = \frac{1}{2}(1-\mu_0^2) \qquad (16)$$

$$D_1^0 = \frac{1}{4}(1+\mu_0)^2 \qquad (17)$$

(11) va (15) tenglamalardan quyidagini topamiz:

$$\sum_{n=2}^{\infty} D_n^0 = \sum_{n=1}^{\infty} D_n^0 - D_1^0 = \frac{1}{12}(1-\mu_0)^2 \qquad (18)$$

D_1^0; $\sum_{n=1}^{\infty} D_n^0$, $\sum_{n=2}^{\infty} D_n^0$ va $\sum_{n=1}^{\infty} D_n^1$ larning θ_0 dan bog'liqliklari keltirilgan.

Bu bog'liqliklar mos ravishda (17), (11), (18) va (12) tenglamalar orqali hisoblaniladi.

Agar D_1^0 D_2^0 D_3^0 va D_1^1 larning $\theta_0 = 150^0$ burchaklar uchun θ_0 dan bog'liqliklarning sonli usullar bilan hisoblangan qiymatlari keltirilgan bo'lsa $\theta_0 \leq 150^0$ qiymat uchun

$$\sum_{n=2}^{\infty} D_n^0 \approx D_2^0 \qquad (19)$$

$$\sum_{n=1}^{\infty} D_n^1 \approx D_1^1 \qquad (20)$$

ya’ni yuqori darajali hadlarni hisobga olmasa bo'ladigan darajada kichik. Quyidagi sodda ifodalarni hosil qilamiz:

$$\langle Y_{1,0}(\Omega(0))Y^*_{1,0}(\Omega(t))\rangle = \frac{3}{4\pi}(D_1^0 + D_2^0 \exp[-\nu_2^0(\nu_2^0+1)D_R t] \qquad (21)$$

$$\langle Y_{1,1}(\Omega(0))Y^{*}_{1,1}(\Omega(t))\rangle = \langle Y_{1,-1}(\Omega(0))Y^{*}_{1,-1}(\Omega(t))\rangle = -\frac{3}{8\pi}D_1^1 \exp[-\nu_1^1(\nu_1^1+1)D_R t] \quad (22)$$

bundan

$$D_1^0 = \frac{1}{4}(1+\mu_0)^2),$$
$$D_2^0 = \frac{1}{22}(1-\mu_0)^2), \quad (23)$$

Bunda cheklangan aylanma diffuziya modeli dipol avtokorrelyasion funksiyalarni hisoblash uchun qo'llaniladi.

Dipol avtokorrelyasion funksiya dielektrik relaksasiya tajribalarida o'lchanadi. Sferik qutb koordinatasida molekula depol momenti $\bar{u}$ quyidagi ko'rinishda yoziladi.

$$u = u_0(\sin\theta\cos\phi\bar{x} + \sin\theta\sin\phi\bar{y} + \cos\theta\bar{z}) \quad (24)$$

Uzluksiz chiziqlar mos ravishda (13), (14), (17) va (19) tenglamalardan

$\sum_{n=1}^{\infty} D_n^0$, $\sum_{n=1}^{\infty} D_n^1$, $\sum_{n=1}^{\infty} D_1^0$ va $\sum_{n=1}^{\infty} D$ lar uchun hisoblandi.

Bu yerda u_0 dipol momentining amplitudasi hisoblanib, sferik garmonikalar orqali dipol momenti quyidagi ko'rinishni oladi.

$$u = \sqrt{\frac{2\pi}{3}}u_0\left\{[Y_{1,-1}(\Omega) - Y_{1,1}(\Omega)]*\bar{x} - i[Y_{1,1}(\Omega) + Y_{1,-1}(\Omega)]\bar{y} + \sqrt{2}Y_{1,0}(\Omega)\bar{z}\right\} \quad (25)$$

Dipol avtokorrelyasion funksiya esa quyidagi ko'rinishni oladi [4].

$$\langle u(0)u^*(t)\rangle = \frac{4\pi}{3}u_0^2\sum_{m=-1}^{1}\langle Y_{l,m}(\Omega(0)Y^{*}_{l,m}(\Omega(t))\rangle \quad (26)$$

Oldingi tenglamalarni (25) va (26) tenglamalarga qo'llab quyidagilarni olamiz.

$$\langle u(0)u^*(t)\rangle = u_0^2(D_1^0 + D_2^0\exp[-\nu_2^0(\nu_2^0+1)D_R t] + + D_1^1\exp[-\nu_1^1(\nu_1^1+1)D_R t]) \quad (27)$$

Shuni aytish mumkinki $\theta_0 = 60^0$ bo'lsa D_1^0 va D_1^1 lar D_2^0 va korrelyasion funksiya faqat bir eksponensial had va baza chizig'i yig'indisidan iborat bo'ladi.

$$\langle u(0)u^*(t)\rangle = \frac{1}{3}u_0^2[(1+\mu_0+\mu_0^2)+(2-\mu_0-\mu_0^2)* *\exp[-\nu_1^1(\nu_1^1+1)D_R t]] = A + B\exp[-\nu_1^1(\nu_1^1+1)D_R t] \quad (28)$$

Cheklangan aylanma diffuziya koeffisiyenti D_R korrelyasion funksiyasining eksponensial hadi orqali aniqlanadi. Ta'kidlash joizki θ_0 ning kamayishidan A/V oshadi va (28) tenglama o'ng tamonidan ikkinchi hadi tez kamayib boradi hamda cheklangan kichik sterjen va kichik konus bazasi chiziqli kengayadi va korrelyasion funksiya esa so'nadi.

Foydalanilgan adabiyotlar

1. McConnell J R 1980 Rotational Brownian Motion and Dielectric Theory (New York: Academic)
2. Burshtein A I and Temkin S I 1994 Spectroscopy of Molecular Rotation in Gases and Liquids (Cambridge: Cambridge University Press)
3. Валиев К. А. Иванов Е. Н., Вращательное броуновское движение. Успехи физических наук., 1973, 109, № 1, 31-64

4. Бойдедаев А. Классик статистик физика. Тошкент, «Ўқитувчи», 2003.