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$^1\Pi$ 态双原子分子中关于 Λ 量子干涉的微分干涉角

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摘要 Sha 等在静态池实验中观察到了转动能量转移中的碰撞量子干涉, 并且计算了决定跃迁散射截面的积分干涉角(*J. Chem. Phys.*, **1995**, **102**: 2772). 由于积分干涉角是微分干涉角的平均效应, 为了得到更精确的信息, 进行了分子束实验. 作者文运用含时微扰的一级波恩近似理论, 提出了衡量干涉程度的 $^1\Pi$ 态双原子分子中关于 Λ 量子干涉的微分干涉角. 利用各向异性相互作用势计算了其干涉角. 得到分子束实验中微分干涉角随实验参数, 包括实验温度、碰撞伴、作用距离和转动量子数变化的关系. 并且讨论了影响干涉角的各种参数. 此理论模型对理解和进行分子束实验是非常重要的.

关键词: 量子干涉, 碰撞诱导转动传能, 微分干涉角, 各向异性相互作用势, 分子束实验

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The Differential Interference Angle of Λ -Related Quantum Interference of $^1\Pi$ -state Diatom

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Abstract Collisional quantum interference (CQI) on rotational energy transfer was observed by Sha *et al.*(*J. Chem. Phys.*, **1995**, **102**: 2772) in static cell, and the integral interference angle which determines the magnitudes of the transition cross sections was measured. To obtain more precise information, the experiment in the molecular beam should be taken, as the integral interference angle is the average effect of the differential interference angle. The differential interference angle of Λ -Related Quantum Interference of $^1\Pi$ -state diatom was presented to measure the degree of coherence, by using the first order Born approximation of time-dependent perturbation theory. The anisotropic Lennard-Jones interaction potential is employed to simulate their interference angles. The relationships of the differential interference angle versus the factors of the experiment in the molecular beam, including experimental temperature, partners, the distance of the interaction and rotational quantum number, are obtained. And the various factors that influence the interference angles are discussed. This theoretical model is important to understand or perform in the experiment of the molecular beam.

Keywords: Quantum interference, Collision-induced rotational energy transfer, Differential interference angle, Anisotropic Lennard-Jones interaction potential, Experiment of the molecular beam

In 1995, Sha *et al.*^[1-2] reported the evidence for collisional quantum interference(CQI) in intramolecular rotational energy transfer within CO $A^1\Pi(\nu=0)\sim e^3\Sigma^-(\nu=1)$ singlet-triplet states in

collision with He, Ne and other partners, following which Chen *et al.*^[3] also observed CQI in $\text{Na}_2A^1\Sigma_u^+(\nu=8)\sim b^3\Pi_{u,1}(\nu=14)$ system in collision with Na ($3s$). The theoretical simulations have been done,

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from which the experiments were further interpreted and supported^[4-8]. In the experiments mentioned above, the collisional partners are atoms, and all the interference angles are less than 90° . However, when HCl as the collisional partner^[9], the interference angles are larger than 90° , which is a significant complementarity and also has been interpreted theoretically^[10-11].

In the mixed electronic states, the CQI was also observed experimentally^[12-18], which results from the Λ splits of open-shell $^1\Pi$ -states diatomic molecules, such as the $^1\Pi$ -state alkali dimers $\text{Li}_2(B^1\Pi_u)$ ^[12-13], Na_2 ^[17], $\text{NaLi}(^1\Pi)$ ^[16] experiments, rotational inelastic collisions of LiH with He ^[17], and collision-induced rotational energy transfer of $\text{CO}(A^1\Pi, \nu)$ with He , Ne and Ar ^[18]. Based on the experimental studies of Ottinger, Bergmann, Zare, and their co-workers^[12-14], Klar^[19], Zare^[20] and Alexander *et al.*^[21] studied the interaction potential for the interaction of a closed-shell atom with a molecule in an electronic state of $^1\Pi$ -symmetry in theory, and the theoretical models of CQI in this case were also presented^[22-23].

The experiments were taken in a static sample cell, so only the integral cross sections and the integral interference angles have been measured. If experiments can be conducted in molecular beams to measure the differential cross section and the differential interference angle, the collisional quantum interference might be observed more precisely, because the integral interference angle is the average effect of the differential interference angle. The ion imaging technique, originally developed by Chandler and Houston^[29], was significantly improved by Eppink and Parker^[30] by using direct velocity mapping technique. Using this technique, Kohguchi^[31] measured fully state-resolved differential cross sections for the inelastic scattering of the open-shell NO molecule by Ar. Recently, the direct 3D time sliced ion velocity imaging method^[32] was developed to measure the product distribution in crossed molecular beam experiment. Similar to the experiments mentioned above, experiments of the $\text{CO}(A^1\Pi(\nu=0) \sim e^3\Sigma^-(\nu=1))$ system in collision with He , Ne and other partners might be performed in the crossed molecular beams, using sliced velocity-mapped ion imaging.

In this paper, to study theoretically proposed experiments in the condition of molecular beams, a theoretical model is presented, based on the time dependent first order Born approximation, taking into account the anisotropic Lennard-Jones interaction potentials, and "straight-line" trajectory approximation. The changing tendencies of differential interference angle of $\text{CO}(A^1\Pi, \nu=3)$

with He , Ne and Ar ^[18] are discussed theoretically. The effects of the factors, including the experimental temperatures, different partners, rotational quantum numbers, and the distance of the interactions, that the interference angles depend on, are obtained.

1 Theoretical approach

1.1 Hamiltonian

For the atom-diatom system, the interaction potential V can be written as^[21],

$$V(R, \theta, \varphi) = \sum_{l, m, k} V_{l, k}(R) \mathbf{D}_{m, k}^l(\Omega) C_m^l(\theta, \varphi) \quad (1)$$

Where R is the orientation from the atom to the mass center of diatom, $\mathbf{D}_{m, k}^l(\Omega)$ is the Wigner D rotational matrix, the Euler angles $\Omega = \alpha, \beta, \gamma$ refer to the space fixed by orientation of the diatom, $C_m^l(\theta, \varphi)$ is a Racah spherical harmonic function, the angles θ, φ describe the orientation of R in the space frame. In the atom and $^1\Pi$ -states diatomic molecules system, $k=0$ or $k=\pm 2$ ^[20, 24]. The evolution of the interaction potential is,

$$V(t) = U^*(t, 0) V U(t, 0) \quad (2)$$

Where $U(t, 0)$ is the time evolution operator,

$$U(t, 0) = \exp(-iH_0 t / \hbar) \quad (3)$$

and where the Hamiltonian H_0 can be written as:

$$H_0 = -\frac{1}{2\mu} \frac{d^2}{dR^2} - \frac{L^2}{2\mu R^2} + H_a + H_e + H_{\text{vib}} + H_{\text{rot}} \quad (4)$$

In this paper, without considering the translational, electronic and vibrational energy transfer, so H_0 in Eq.(4) can be simplified to rotational energy and the rotational kinetic energy of the atom about the diatom, $H_0 = -\frac{L^2}{2\mu R^2} + H_{\text{rot}}$. To simplify the discussion,

without considering the rotational kinetic energy of the atom about the diatom, and for the $^1\Pi$ -states diatomic molecules,

$$H_0 = \omega \eta = 2\pi \hbar c [B^S J(J+1) - 2\Omega' \Lambda + \Lambda^2] \quad (5)$$

Where $\Lambda=1$ and $\Omega' = \Omega = \pm 1$ or $\Omega' = -\Omega = \pm 1$.

1.2 Wave function for the $^1\Pi$ -state diatom molecule

For a $^1\Pi$ -state diatomic molecule, the wave functions are of definite parity, which may be written as^[33],

$$|JM\varepsilon\rangle = \frac{1}{\sqrt{2}} [|JM|\Omega\rangle + \varepsilon |JM, -\Omega\rangle] \quad (6)$$

where J is the angular momentum quantum number of the diatom, M is the projection of J along the space-fixed Z -axis, $\Omega = \Lambda = \pm 1$ is the projection of total angular momentum on the molecular frame, and $\varepsilon = \pm 1$. The quantity ε will be designated as the parity index. Within the spectroscopic nomenclature, the $\varepsilon = +1$ levels

are designated as e and the $\varepsilon=-1$ levels as $f^{[34]}$. The rotational wave function $|JM\Omega\rangle$ which appears in Eq.(6) can be written as a rotational matrix element^[33], namely

$$|JM\Omega\rangle=[(2J+1)/8\pi^2]^{1/2} D'_{M\Omega}(\alpha\beta\gamma) \quad (7)$$

Considering the interaction between a $^1\Pi$ diatomic molecule and a spherical atom in a singlet state, the total wave function is usually expanded in terms of eigenfunctions of the total angular momentum ζ , which are defined by^[34]

$$|J\Omega\varepsilon\zeta s\rangle=\sum_{MM_L} \langle JMLM_L|\zeta s\rangle|LM_L\rangle|JM\varepsilon\rangle \quad (8)$$

Where s is the space-frame projection of ζ , L is the orbital angular momentum of the atom-molecule pair with space-frame projection M_L , and $|LM_L\rangle$ is a spherical harmonic^[21].

1.3 The transition matrix element and probability

According to the first order Born approximation of time dependent perturbation theory, considering the product of three rotation matrix element and spherical harmonics and the relationship between $3j$ symbols and $6j$ symbols, the transition matrix element is^[26],

$$\begin{aligned} \langle J'\Omega'\varepsilon'\zeta s|V(t)|J\Omega\varepsilon\zeta s\rangle &= (-1)^{J'+\varepsilon-4A} [(2J+1)(2J'+1)(2L+1)(2L'+1)]^{1/2} \cdot \\ &\sum_l \frac{1}{2} [1+\varepsilon\varepsilon'(-1)^{J'+J+l}] \times \begin{pmatrix} L' & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} J & L & \zeta \\ L' & J' & l \end{Bmatrix} \begin{Bmatrix} J' & l & J \\ 1 & 0 & -1 \end{Bmatrix} \cdot \\ &\exp(i\omega_{J'J}^{\Delta E=0} t) V_{l,0}[R(t)] + \varepsilon \begin{pmatrix} J' & l & J \\ -1 & 2 & -1 \end{pmatrix} \exp(i\omega_{J'J}^{\Delta E=2} t) V_{l,2}[R(t)] \end{aligned} \quad (9)$$

The unpolarized transition probability can be written as^[25],

$$P_{J'J} = \frac{1}{(2J+1)} \sum_{l'l'} \left| \frac{1}{i\eta} \int_{-\infty}^{\infty} \langle J'\Omega'\varepsilon'\zeta s|V(t)|J\Omega\varepsilon\zeta s\rangle dt \right|^2 \quad (10)$$

Introducing Eq.(9) into Eq.(10), one can obtain an explicit transition probability formula for the $J \rightarrow J'^{[26]}$,

$$P_{J'J} = P_{J'J}^{\Delta E=0} + P_{J'J}^{\Delta E=2} + 2\varepsilon \sum_l [(P_{J'J}^{\Delta E=0})_l]^{1/2} [(P_{J'J}^{\Delta E=2})_l]^{1/2} \quad (11)$$

Eq.(12) also can be written as,

$$P_{J'J} = P_{J'J}^{\Delta E=0} + P_{J'J}^{\Delta E=2} + 2\varepsilon (P_{J'J}^{\Delta E=0} P_{J'J}^{\Delta E=2})^{1/2} \cos\theta^D \quad (12)$$

With the differential interference angle,

$$\cos\theta^D = \frac{\sum_l [(P_{J'J}^{\Delta E=0})_l]^{1/2} [(P_{J'J}^{\Delta E=2})_l]^{1/2}}{(P_{J'J}^{\Delta E=0} P_{J'J}^{\Delta E=2})^{1/2}} \quad (13)$$

And if only the rotational energy transfer is considered^[26],

$$\omega_{J'J} = 2\pi c B [J'(J'+1) - 2\Omega'\Lambda + \Lambda^2] - 2\pi c B [J(J+1) - 2\Omega\Lambda + \Lambda^2] \quad (14)$$

For the $^1\Pi$ -state diatom, $\Lambda=1$ and $\Omega'=\Omega=\pm 1$ or $\Omega'=-\Omega=\pm 1$.

The experiment of CO $A^1\Pi(\nu=3)$ system in collision with He, Ne and Ar has been done by Sun *et al.*^[18] in a static sample cell. However, the differential interference angle, which has

been derived for the partners with uniform collision velocity, is not appropriate to deal with the static sample cell experiments in which the gas species have the Maxwell-Boltzmann velocity distribution. In this case, Sharma *et al.*^[36] have derived a formula to get velocity-averaged probability,

$$P_{AV} = \int_0^{\infty} P(\nu) \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu / \int_0^{\infty} \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu = 2\left(\frac{\mu}{kT}\right)^2 \int_0^{\infty} P(\nu) \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu \quad (15)$$

and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of the collision system, T is

the temperature of the static cell. Now, the velocity-averaged cross-sections can be obtained by introducing Eq.(11) or (12) into Eq.(15) to get $P_{J'J}(AV)$ and then the $P_{J'J}(AV)$ into Eq.(13):

$$\cos\theta_{AV}^D = \frac{\int_l \sum_l [(P_{J'J}^{\Delta E=0})_l]^{1/2} [(P_{J'J}^{\Delta E=2})_l]^{1/2} \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu}{\left(\int_l \sum_l (P_{J'J}^{\Delta E=0})_l \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu \right)^{1/2} \left(\int_l \sum_l (P_{J'J}^{\Delta E=2})_l \nu^3 \exp\left(-\frac{\mu\nu^2}{2kT}\right) d\nu \right)^{1/2}} \quad (16)$$

2 Results and discussions

In the following sections, we detailed the relationships of the differential interference angle versus the factors of the experiment in the molecular beam. The differential interference angle measures the degree of coherence, which originates from the difference between the two Λ -related collision potential energy surfaces. To simplify the discussion, we adopt the anisotropic Lennard-Jones interaction ($l \leq 2$) in the space frame,

$$V_A(R, \theta, \varphi) = V_1(R) \sum_m [a_{1,0} D_{m,0}^1(\alpha, \beta, \gamma) C_m^1(\theta, \varphi)] + V_2(R) \sum_{m,k} [a_{2,k} D_{m,k}^2(\alpha, \beta, \gamma) C_m^2(\theta, \varphi)] \quad (17)$$

With^[25],

$$V_1(R) = 4\varepsilon [(\rho/R)^{12} - (\rho/R)^7] \quad (18)$$

$$V_2(R) = 4\varepsilon [(\rho/R)^{12} - (\rho/R)^6] \quad (19)$$

Where $a_{l,k}$ is the anisotropic parameters, ρ is the distance at which $V(R)=0$, ε is the depth of the potential-well, which is a measure of how strongly the molecules attract each other.

Simply, we only consider V_2 , then the differential interference angle can be written as,

$$\cos\theta_{AV}^D = \frac{\langle A \rangle}{\langle B \rangle^{1/2} \langle C \rangle^{1/2}} \quad (20)$$

where

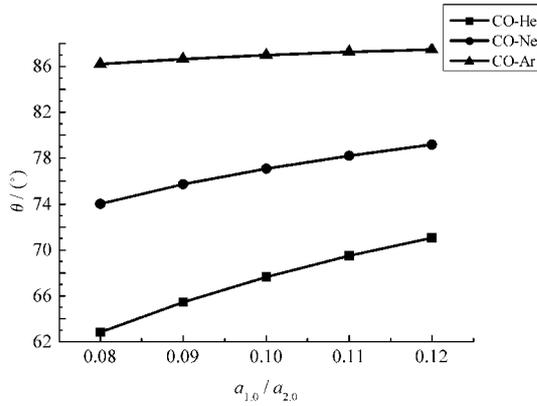


Fig.1 Differential interference angles (θ) with the ratio range of $a_{1,0} / a_{2,0}$ at $b=b_{\min}$, $J=7$, $T=181$ K

$$\langle A \rangle = \int \left| \frac{\rho^{12}}{b^{11}} F_d(x^{\Delta l \pm 0}) - \frac{\rho^6}{b^5} F_3(x^{\Delta l \pm 0}) \right| \times \left[\frac{\rho^{12}}{b^{11}} F_d(x^{\Delta l \pm 2}) - \frac{\rho^6}{b^5} F_3(x^{\Delta l \pm 2}) \right] \nu \exp\left(\frac{-\mu \nu^2}{2kT}\right) d\nu \quad (21)$$

$$\langle B \rangle = \frac{(a_{1,0})^2 \sum_{L'L'} (2L'+1) \begin{pmatrix} L' & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} J & L & \zeta \\ L' & J' & l \end{pmatrix}^2 \begin{pmatrix} J' & l & J \\ -1 & 0 & 1 \end{pmatrix}^2}{(a_{2,0})^2 \sum_{L'L'} (2L'+1) \begin{pmatrix} L' & 2 & L \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} J & L & \zeta \\ L' & J' & 2 \end{pmatrix}^2 \begin{pmatrix} J' & 2 & J \\ -1 & 0 & 1 \end{pmatrix}^2} \times \frac{\sigma^6}{\nu b^{11}}$$

$$F_6(x^{\Delta l \pm 0}) - \frac{1}{\nu b^5} F_{7/2}(x^{\Delta l \pm 0}) \left| + \frac{\sigma^6}{\nu b^{11}} F_6(x^{\Delta l \pm 0}) - \frac{1}{\nu b^5} F_3(x^{\Delta l \pm 0}) \right|^2 \quad (22)$$

$$\langle C \rangle = \int \left[\frac{\rho^{12}}{b^{11}} F_d(x^{\Delta l \pm 2}) - \frac{\rho^6}{b^5} F_3(x^{\Delta l \pm 2}) \right]^2 \nu \exp\left(\frac{-\mu \nu^2}{2kT}\right) d\nu \quad (23)$$

In Eq.(22), the ratio of $a_{1,0} / a_{2,0}$ for CO in collision with He, Ne and Ar is $0.08 \leq a_{1,0} / a_{2,0} \leq 0.12$ ^[28].

From Eq.(20)~(23), one can obtain the differential interference angle for $J'=J \pm 1$. For example, when $J'=J+1$, the differential interference angle can be calculated quantitatively and some of the derivations can be referenced in Appendix. (the needed parameters of the theoretical calculation are listed in Table 1), and four conclusions can be obtained:

1) As presented in Fig.1, resulting from the increase of $a_{1,0} / a_{2,0}$, the differential interference angle increases, so the quantum interference effect of rotational energy transfer decreases. When $a_{1,0} / a_{2,0}=0$, the interference is the complete interference.

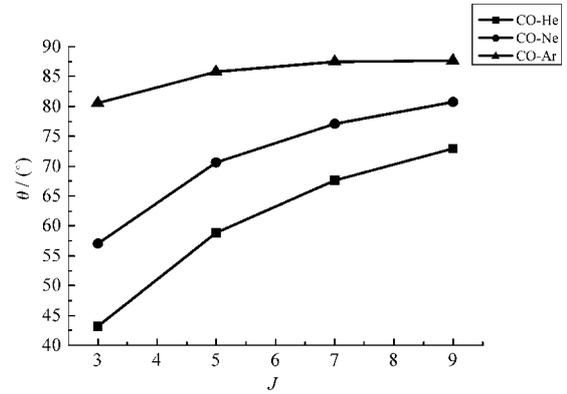


Fig.2 Differential interference angles (θ) with rotational quantum numbers (J) at $b=b_{\min}$, $a_{1,0}/a_{2,0}=0.1$ and $T=181$ K

2) The curve given in Fig.2 exhibits the changing tendency of the differential interference angles (θ), which are consistent with the experiment^[1-2]. Therefore, we give the explanation of the differential interference angles values as: the collisional interaction increases in the condition of rotational quantum numbers' increasing, and the spin-orbit mixed states will decouple due to the different energy level shifts of the spin-orbit conserving transition and the spin-orbit changing transition induced by the collision perturbation. As a result of decoupling, the mixing degree of corresponding wave functions will become much smaller than that of the isolated molecule and the interference effect will become weaker as well.

3) With the increase of experimental temperature, the differential interference angle (θ) decreases for He and Ne, so the quantum interference effect of rotational energy transfer increases. But for Ar, the changing tendency of differential interference angle with experimental temperature is not monotonic, as presented in Fig.3.

We suggest that the orbit angular momentum and the relative velocity depend on the experimental temperature. The former influences the electrostatic interaction potential V between the atom and diatom. The mixing degree of corresponding wave functions will become much bigger than that of the isolated molecule due to the increasing of the temperature, and the inter-

Table 1 Parameters needed in the theoretical calculation

Collision system	Reduced mass (a.m.u)	10 σ / nm	10 b_{\min} / nm	L			B / cm ⁻¹
				$T=77$ K	$T=181$ K	$T=253$ K	
CO-He	3.5 ^[4]	2.56 ^[24]	2.9 ^[25]	11	17	20	1.5346 ^[26]
CO-Ne	11.75 ^[6]	2.75 ^[24]	3.1 ^[6]	22	33	39	1.5346 ^[26]
CO-Ar	17.5 ^[6]	3.41 ^[24]	3.5 ^[6]	30	45	54	1.5346 ^[26]

B : rotation constant; $L=\mu \nu b / \eta = \mu b / \eta \sqrt{8kT/\pi \mu}$

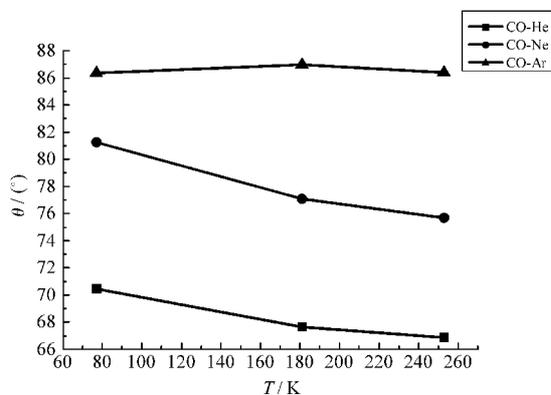


Fig.3 Differential interference angles (θ) with experimental temperatures T at $b=b_{\min}$, $J=7$ and $a_{1,0}/a_{2,0}=0.1$

ference effect will become stronger as well. However the latter not only affects the duration of collision but the ability of the impact parameter to overcome interactive potential barrier. Therefore, it can be said that the higher relative velocity, the shorter duration of collision and the higher energy to access to each other easier, which will decrease the interference. And the competition between them was supposed to determine the final temperature-dependent relationships.

4) In the last section, we will discuss the relation between the differential interference angle and the impact parameter. The nonmonotonic changing tendencies for all partner are illustrated in Fig.4. Two main aspects, we think, contribute to it: a) the probability of rotational energy transfer and interference will increase with the elongation of the duration of collision, and the impact parameter just plays a key role in affecting the duration. b) the energy interval has a large connection with the impact parameter, and larger impact parameter will bring an opposite effect to the interference when contrasted to aspect a. In Fig.4, we have taken the two aspects' element and the curves in it are the general effects.

Besides, we also get the information which is consistent with the experiment^[12] and the calculated values of the differential interference angles that with the increase of reduced mass, the differential interference angle, and hence the quantum interference effect of rotational energy transfer decrease. We suspect that it is closely related to the orbit angular momentum mentioned above.

3 Conclusions

Collisional quantum interference of $^1\Pi$ -state diatomic molecules on rotational energy transfer, which originates from

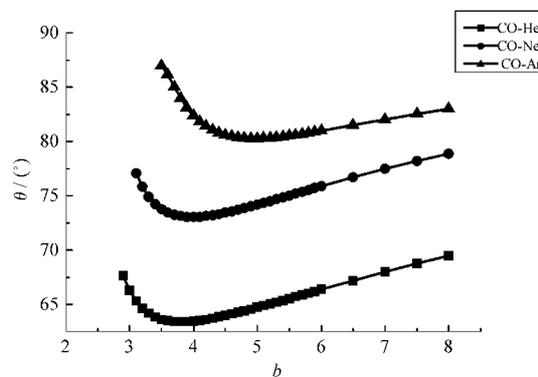


Fig.4 Differential interference angles (θ) with impact parameter b at $J=7$, $a_{1,0}/a_{2,0}=0.1$ and $T=181$ K

the difference between the two Λ -related collision potential energy surfaces, has been studied theoretically. Based on the time dependent first order Born approximation, taking into account the anisotropic Lennard-Jones interaction potentials and "straight-line" trajectory approximation, the factors that the differential interference angle depends on are obtained, and the changing tendency of the interference with them is discussed.

Appendix:

$$\begin{pmatrix} J' & l & J \\ -1 & 0 & 1 \end{pmatrix}^2 = \frac{2(-1)^{-2l}J(2+J)}{(1+2J)(2+2J)(3+2J)} \quad (\text{A.1})$$

$$\begin{pmatrix} L' & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{2(-1)^{-2l}(1+L)^2}{(1+2L)(2+2L)(3+2L)} \quad (\text{A.2})$$

$$\left\{ \begin{matrix} J & L & \xi \\ L' & J' & l \end{matrix} \right\}^2 = \frac{(-1)^{-4l}J(-2+2L)}{(2+2J)(3+2J)L(1+2L)} \quad (\text{A.3})$$

where we set $\xi=J+L-1$.

$$\begin{pmatrix} J' & 2 & J \\ -1 & 0 & 1 \end{pmatrix}^2 = \frac{12(-1)^{-2l}(2+J)}{(1+2J)(2+2J)(3+2J)(4+2J)} \quad (\text{A.4})$$

$$\begin{pmatrix} L' & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{3(-1)^{2l}(-1+L)^2L}{(-3+2L)(-2+2L)(-1+2L)(1+2L)} \quad (\text{A.5})$$

$$\left\{ \begin{matrix} J & L & \xi \\ L' & J' & l \end{matrix} \right\}^2 = \frac{2(-1)^{-4l}(2J+2L)}{(3+2J)(4+2J)L(1+2L)} \quad (\text{A.6})$$

where we set $\xi=J+L-1$.

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