

Simulating reaction of $\text{Ne}^* + \text{OCS}$ collision

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1 Improved potential interpolations

Potential is now fitted to the force field instead of interpolation, because of smoothness issues. Gamma potentials now have correct vanishing derivatives for angles 0 and π .

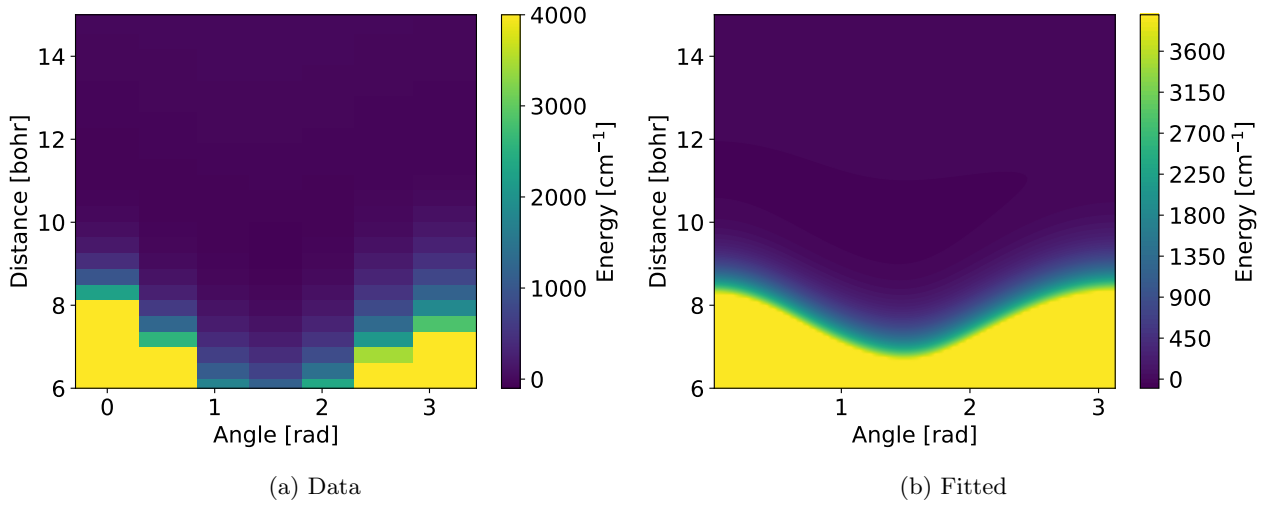


Figure 1: Fitting of intermolecular potential

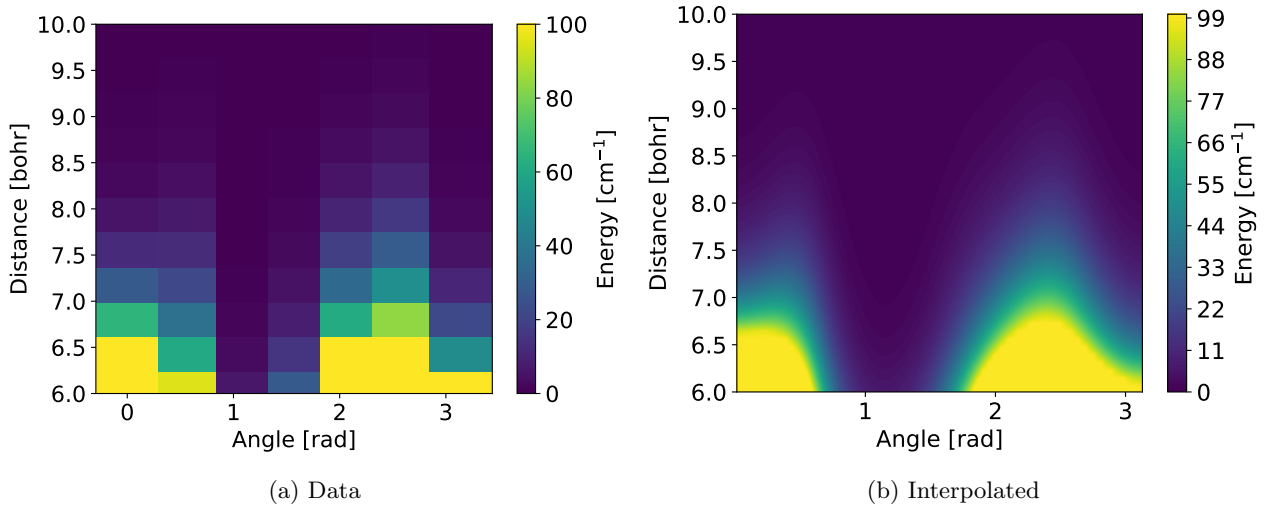


Figure 2: Interpolation of XII gamma potential

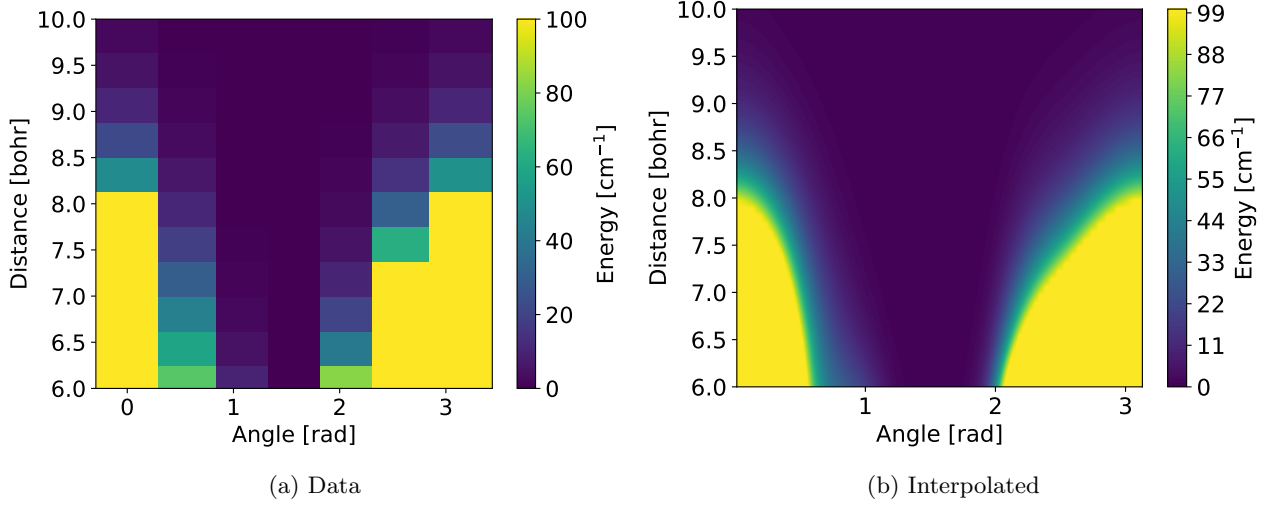


Figure 3: Interpolation of $B\Sigma$ gamma potential

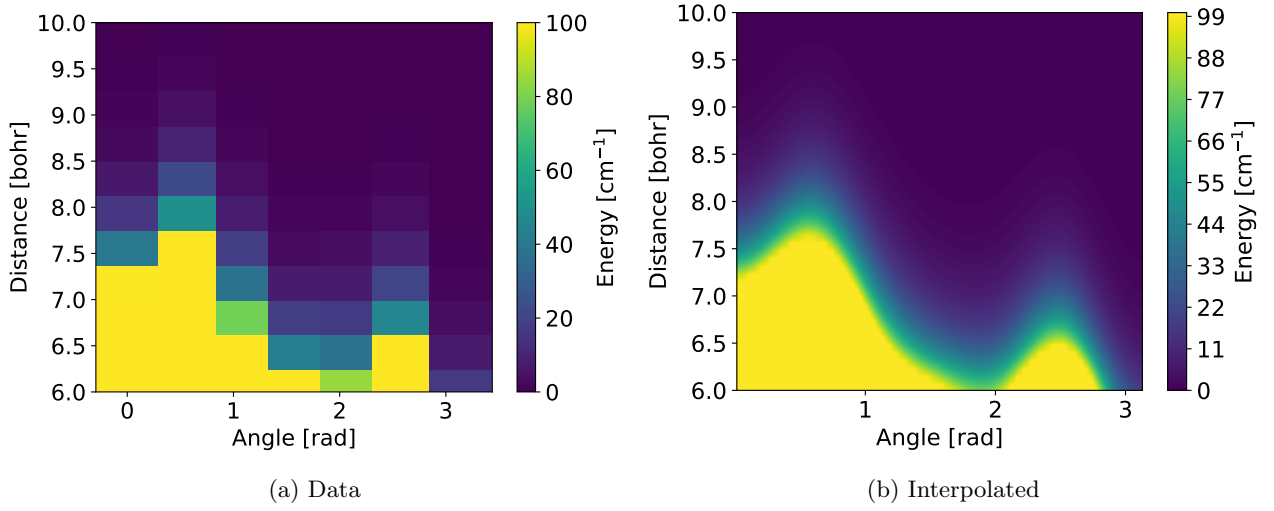


Figure 4: Interpolation of AII gamma potential

2 Reaction rate ratios dependence on force field scalings

Scaling the parameters of the force field (fitted as well as with theoretical values) did not change the reaction rate ratio from value of 1. As an example we show carbo attraction strength scaling.

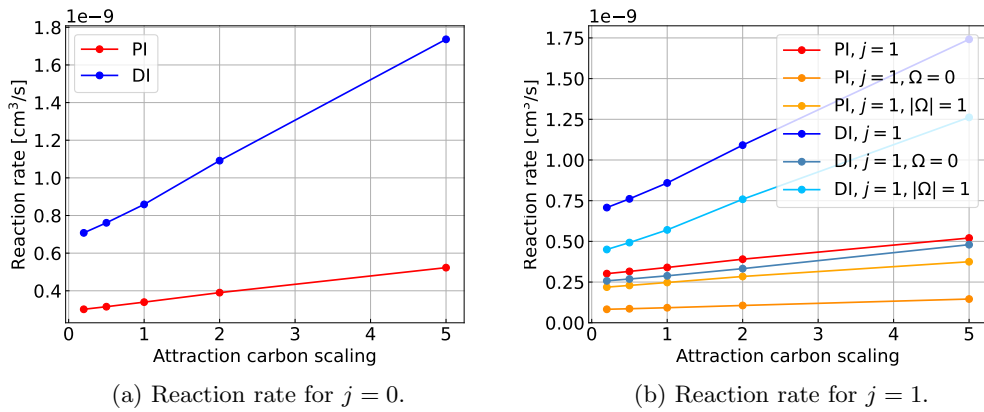


Figure 5: Calculated reaction rates dependence on carbon attraction strength.

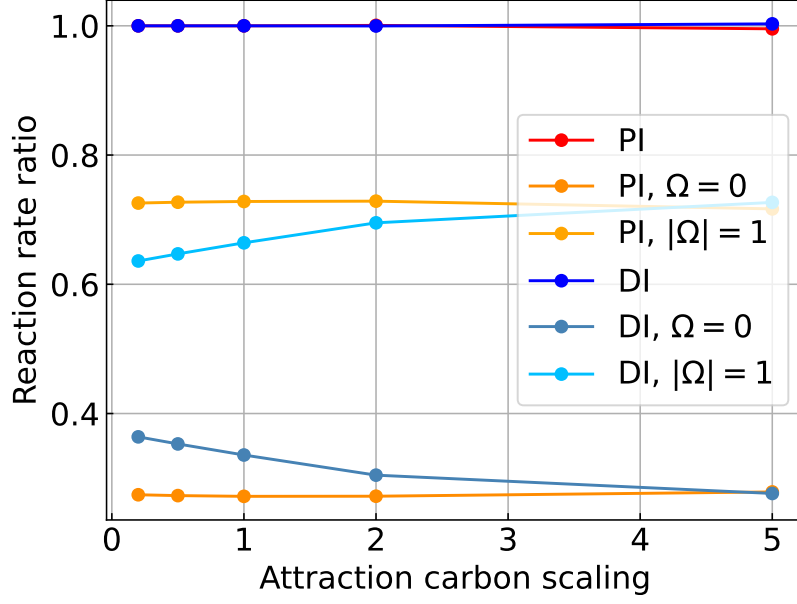


Figure 6: Calculated reaction rate ratio between $j = 1$ and $j = 0$, dependence on carbon attraction strength.

3 Truth tests for coriolis effect inclusion

To test coriolis effect inclusion, we compare the ground state energy of the modified harmonic oscillator using different reference frames.

The system defined by the space-fixed Hamiltonian is

$$\hat{H} = -\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{\hat{L}^2}{2\mu R^2} + V(R, \theta), \quad (1)$$

this frame is equivalent to body-fixed frame that we use for calculations with rotational constant $B = 0$, the Hamiltonian is

$$\hat{H} = -\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{(\hat{J} - \hat{j})^2}{2\mu R^2} + V(R, \theta). \quad (2)$$

The conserved quantities for the first system is the angular momentum projection number m_l , in case of the body-fixed frame the conserved quantity is the total angular momentum J .

We use following harmonic oscillator potential

$$V(r, \theta) = \frac{\mu\omega^2}{2}(r - r_0)^2. \quad (3)$$

The calculated ground state energy of the space-fixed Hamiltonian is equal to ω for projection $m = 0$. For the body-fixed Hamiltonian the calculated ground state for $J = 2$ is also ω with coriolis effect and 1.08ω if we neglect the coriolis effect and with $\Omega_{\text{init}} = 0$.

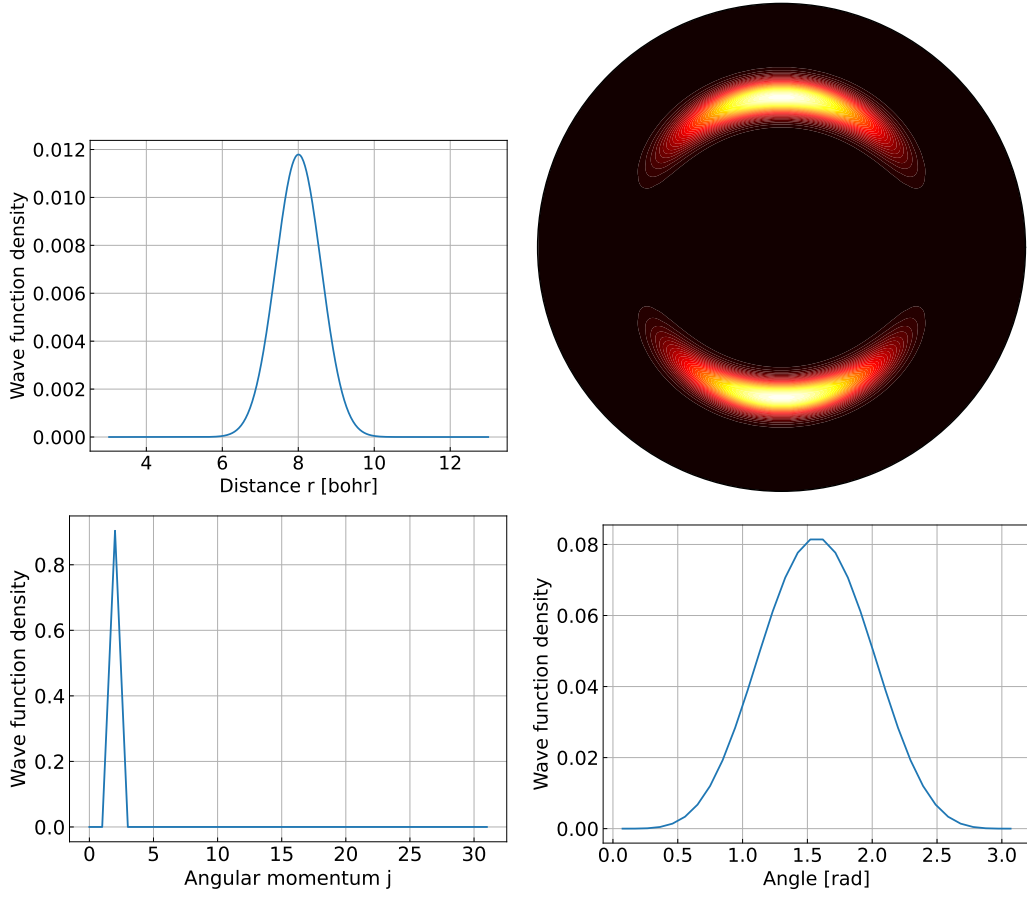


Figure 7: Wave function densities for calculated ground state for $J = 2$ without coriolis effect.

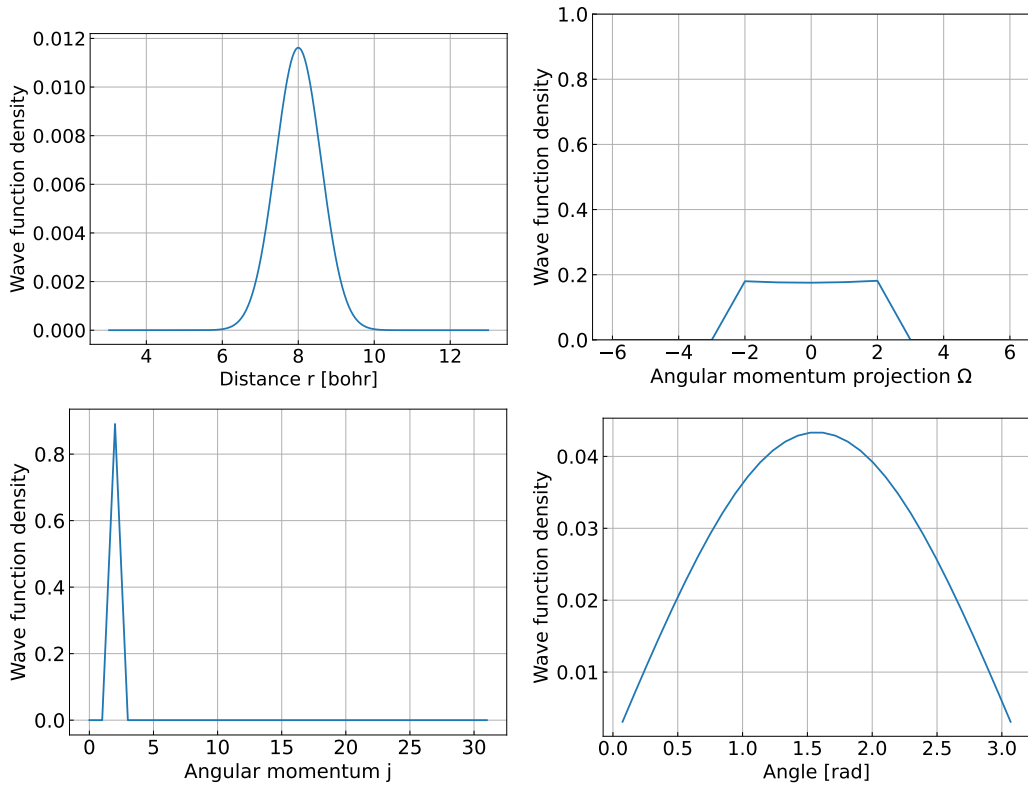


Figure 8: Wave function calculated ground state for $J = 2$ with coriolis effect.

For the potential of the form $V(r, \theta, \phi)$ the space-fixed Hamiltonian doesn't have any conserved angular

numbers, however in body-fixed frame we have still J conserved. It can be deduced that in the case of $B = 0$, J gives additional infinite degeneracy. Because of that, for every conserved J , the ground state is ω , however it is only achievable with the inclusion of the coriolis effect.

Additionally, we test the direct effect of the coriolis effect by multiplying the coriolis term by a factor, results are shown below.

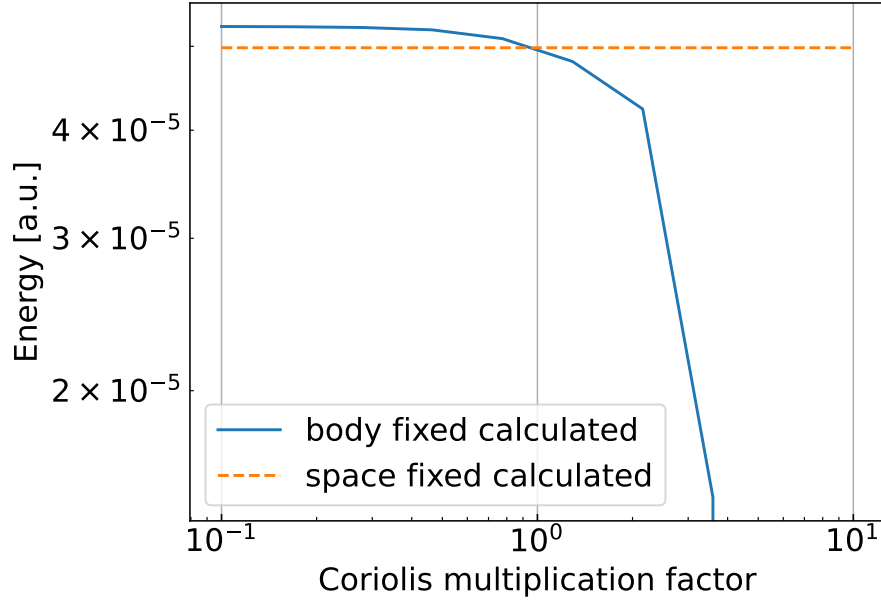


Figure 9: Calculated ground state energy dependence on the coriolis multiplication factor.

4 Reaction rate dependence on the coriolis effect body-fixed projection cutoff

Animations of collision with high Ω_{\max} showed that the mixing of the total projection is up to $\Omega = 45$. However reaction rate calculations converge for $\Omega_{\max} = 2$ as shown below.

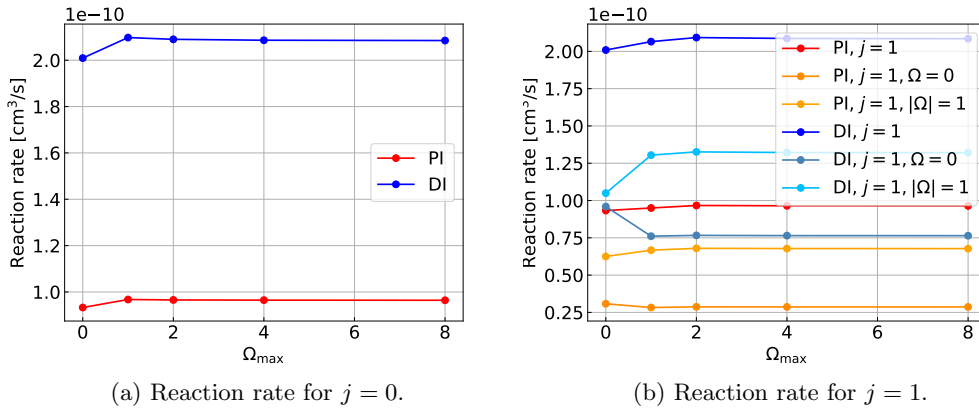


Figure 10: Calculated reaction rates dependence on Ω_{\max} .

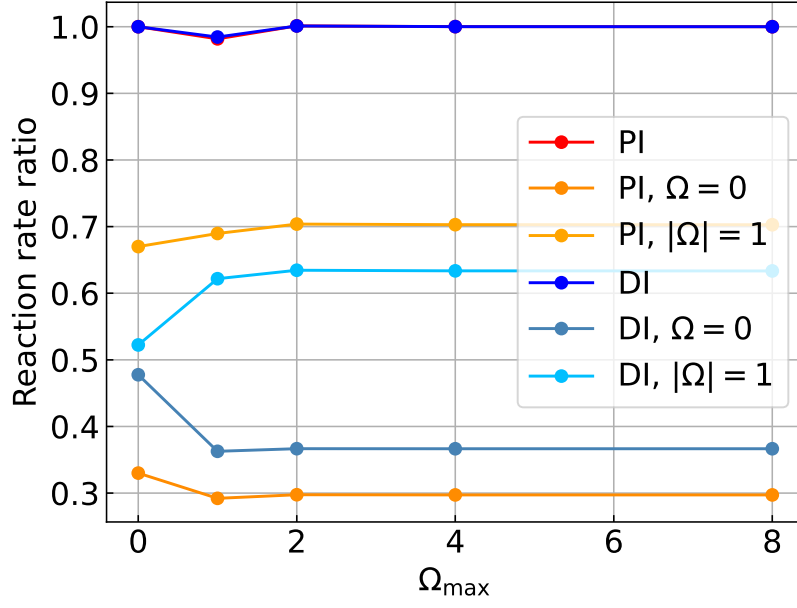


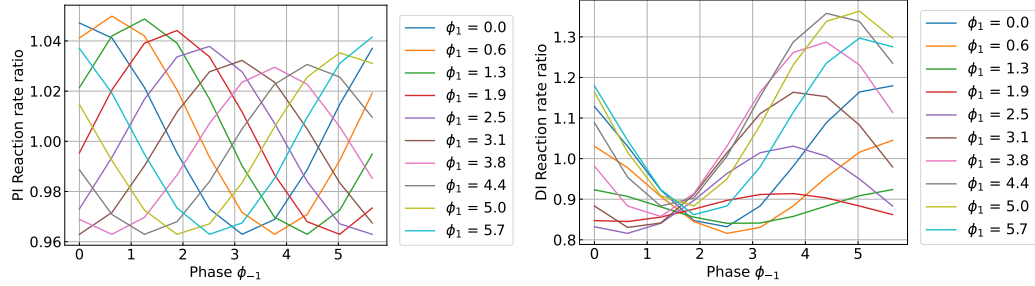
Figure 11: Calculated reaction rate ratio between $j = 1$ and $j = 0$, dependence on Ω_{\max} .

5 Superposition reaction rate

For the initial state $j = 1$ being the superposition of initial body-fixed projections

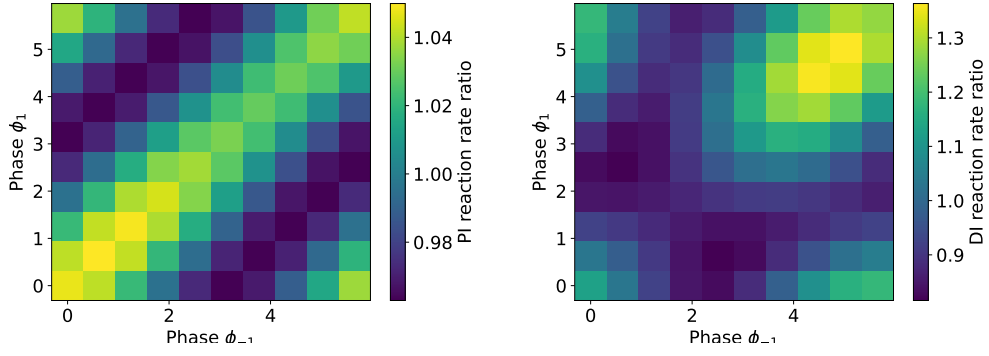
$$|\psi\rangle = \frac{1}{\sqrt{3}} (e^{i\phi_{-1}} |-1\rangle + |0\rangle + e^{\phi_1} |1\rangle), \quad (4)$$

the reaction rate for different initial relative phases is shown below.



(a) Penning ionization reaction rate ratios for different relative phases. (b) Dissociative ionization reaction rate ratios for different relative phases.

Figure 12: Reaction rate ratios for different relative phases.



(a) Penning ionization reaction rate ratios for different relative phases. (b) Dissociative ionization reaction rate ratios for different relative phases.

Figure 13: Reaction rate ratios for different relative phases.

Notice that the reaction rate ratio changes from 1 far more for DI channel than the PI channel, which is consistent with the results of the experiment.

We additionally calculated, for every relative phases, the alignment evolution as shown below.

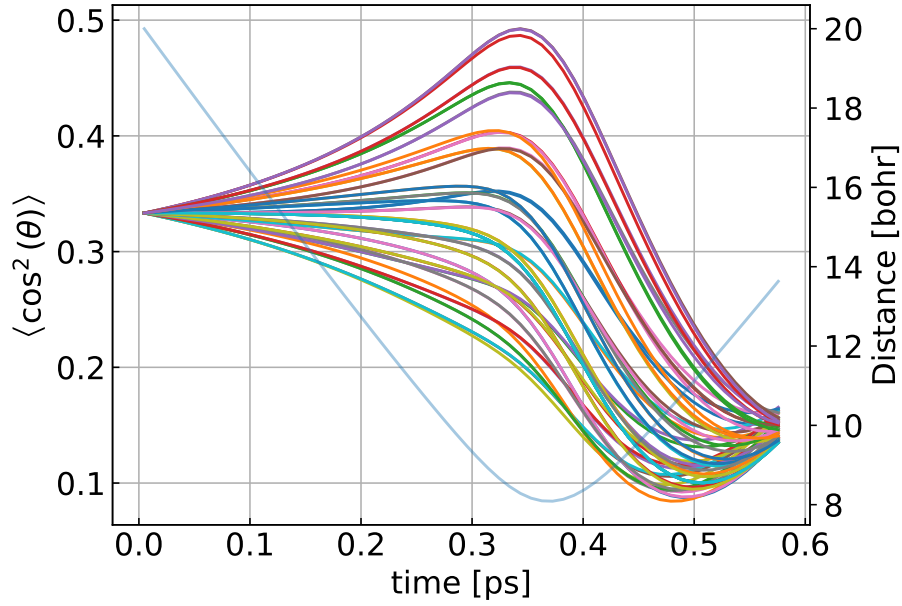


Figure 14: Calculated alignments during the collision for different relative phases.

This brings the idea that after the OCS free flight there is a coherent relative phase in the case of $j = 1$, this relative coherence might be a result of the geometry of the experimental setup or various electric/magnetic fields.