Supplemental Information for:

"Mixed Quantum/Classical Theory for Rotational Energy Exchange in Symmetric-Top-Rotor + Linear-Rotor Collisions and a Case Study of $ND_3 + D_2$ System"

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1. The derivation of expression for transition matrix elements, Eq. (14) in the main text

The wavefunction that describes the motion of the symmetric top + diatom can be expressed analytically as:

$$\Psi_{nm}(\Lambda_1,\Lambda_2) = \sqrt{\frac{2j_1+1}{8\pi^2}}\sqrt{\frac{1}{2\left(1+\delta_{k_1,0}\right)}} \times \sum_{m_1=-j_1}^{+j_1} C^{j,m}_{j_1,m_1,j_2,m-m_1}\left[D^{j_1\,*}_{m_1,k_1}(\Lambda_1) + \epsilon D^{j_1\,*}_{m_1,-k_1}(\Lambda_1)\right]Y^{j_2}_{m-m_1}(\Lambda_2) \qquad (S1)$$

The multidimensional potential can be expanded over a set of suitable angular functions $\tau_{\lambda_1\mu_1\lambda_2\lambda}(\Lambda_1,\Lambda_2)$ with expansion coefficients $\upsilon_{\lambda_1\mu_1\lambda_2\lambda}(R)$ computed by numerical quadrature.

$$V(R,\Lambda_1,\Lambda_2) = \sum_{\lambda_1\mu_1\lambda_2\lambda} \upsilon_{\lambda_1\mu_1\lambda_2\lambda}(R) \times \tau_{\lambda_1\mu_1\lambda_2\lambda}(\Lambda_1,\Lambda_2) \qquad (S2)$$

where,

$$\tau_{\lambda_1\mu_1\lambda_2\lambda}(\Lambda_1,\Lambda_2) = \sqrt{\frac{2\lambda_1+1}{4\pi}} \sum_{\eta=-\min(\lambda_1,\lambda_2)}^{+\min(\lambda_1,\lambda_2)} C^{\lambda,0}_{\lambda_1,\eta,\lambda_2,-\eta}\left[D^{\lambda_1\,*}_{\eta,\mu_1}(\Lambda_1) + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda} D^{\lambda_1\,*}_{\eta,-\mu_1}(\Lambda_1)\right]Y^{\lambda_2}_{-\eta}(\Lambda_2) \qquad (S3)$$

The potential coupling matrix $M^{n''}_{n'}(R)$ can be expressed as follows:

$$M^{n''}_{n'}(R) = \left\langle \Psi_{n''m}(\Lambda_1,\Lambda_2) \middle| V(R,\Lambda_1,\Lambda_2) \middle| \Psi_{n'm}(\Lambda_1,\Lambda_2) \right\rangle \qquad (S4)$$

Here $\Psi_{n''m}(\Lambda_1,\Lambda_2)$ and $\Psi_{n'm}(\Lambda_1,\Lambda_2)$ represents wavefunctions of final and initial states of the molecule.

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To compute state-to-state matrix elements we have to substitute Eq. (S2) into Eq. (S3), followed by the substitution of Eqs. (S1-S2) on to as Eq. (S4) :

$$\left\langle \Psi_{n^{''}m}(\Lambda_1,\Lambda_2) \middle| V(R,\Lambda_1\Lambda_2) \middle| \Psi_{n^{'}m}(\Lambda_1,\Lambda_2) \right\rangle =$$

$$= \sqrt{\frac{2j_1^{''}+1}{8\pi^2}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{''},0}\right)}}\sqrt{\frac{2j_1^{'}+1}{8\pi^2}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{'},0}\right)}}\sum_{m_1^{'}=-j_1^{'}}^{+j_1^{'}} C_{j_1^{'},m_1^{'},j_2^{'},m-m_1^{'}}^{j^{'},m}\sum_{m_1^{''}=-j_1^{''}}^{+j_1^{''}} C_{j_1^{''},m_1^{''},j_2^{''},m-m_1^{''}}^{j^{''},m}$$

$$\times \sum_{\lambda_1\mu_1\lambda_2\lambda} \upsilon_{\lambda_1\mu_1\lambda_2\lambda}(R)\sqrt{\frac{2\lambda_1+1}{4\pi}}\sum_{\eta=-\min(\lambda_1,\lambda_2)}^{+\min(\lambda_1,\lambda_2)} C_{\lambda_1,\eta,\lambda_2,-\eta}^{\lambda,0}\left\langle Y_{m-m_1^{''}}^{j_2^{''}}(\Lambda_2) \middle| Y_{-\eta}^{\lambda_2}(\Lambda_2) \middle| Y_{m-m_1^{'}}^{j_2^{'}}(\Lambda_2)\right\rangle$$

$$\times \left[\begin{aligned} &\left\langle D_{m_1^{''},k_1^{''}}^{j_1^{''}*}(\Lambda_1) \middle| D_{\eta,\mu_1}^{\lambda_1*}(\Lambda_1) \middle| D_{m_1^{'},k_1^{'}}^{j_1^{'}*}(\Lambda_1)\right\rangle + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}\left\langle D_{m_1^{''},k_1^{''}}^{j_1^{''}*}(\Lambda_1) \middle| \cdots \right. \\ &+\epsilon^{'}\left\langle D_{m_1^{''},k_1^{''}}^{j_1^{''}*}(\Lambda_1) \middle| D_{\eta,\mu_1}^{\lambda_1*}(\Lambda_1) \middle| D_{m_1^{'},-k_1^{'}}^{j_1^{'}*}(\Lambda_1)\right\rangle + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}\left\langle D_{m_1^{''},k_1^{''}}^{j_1^{''}*}(\Lambda_1) \cdots \right. \\ &+\epsilon^{''}\left\langle D_{m_1^{''},-k_1^{''}}^{j_1^{''}*}(\Lambda_1) \middle| D_{\eta,\mu_1}^{\lambda_1*}(\Lambda_1) \middle| D_{m_1^{'},k_1^{'}}^{j_1^{'}*}(\Lambda_1)\right\rangle + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}\left\langle D_{m_1^{''},-k_1^{''}}^{j_1^{''}*}(\Lambda \cdots \right. \\ &+\epsilon^{'}\epsilon^{''}\left\langle D_{m_1^{''},-k_1^{''}}^{j_1^{''}*}(\Lambda_1) \middle| D_{\eta,\mu_1}^{\lambda_1*}(\Lambda_1) \middle| D_{m_1^{'},-k_1^{'}}^{j_1^{'}*}(\Lambda_1)\right\rangle + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}\left\langle D_{m_1^{''},-k_1^{''}}^{j_1^{''}*}(\cdots \right. \end{aligned} \right.$$

For the integrals of spherical harmonics, the following equality can be employed [1]:

$$\left\langle Y_{m_3}^{l_3} \middle| Y_{m_2}^{l_2} \middle| Y_{m_1}^{l_1} \right\rangle = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}} C_{l_1,0,l_2,0}^{l_3,0} C_{l_1,m_1,l_2,m_2}^{l_3,m_3} \qquad (S5)$$

For the integrals of Wigner D-functions, the following equality can be employed [1]:

$$\left\langle D_{m_3m_3^{'}}^{l_3*} \middle| D_{m_2m_2^{'}}^{l_2*} \middle| D_{m_1m_1^{'}}^{l_1*} \right\rangle = \frac{8\pi^2}{2l_3+1} C_{l_1,m_1,l_2,m_2}^{l_3,m_3} C_{l_1,m_1^{'},l_2,m_2^{'}}^{l_3,m_3^{'}} \qquad (S6)$$

With these, we have:

$$M^{n''}_{n'}(R) = \sqrt{\frac{2j_1^{''}+1}{8\pi^2}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{''},0}\right)}}\sqrt{\frac{2j_1^{'}+1}{8\pi^2}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{'},0}\right)}}\sum_{m_1^{'}=-j_1^{'}}^{+j_1^{'}} C^{j^{'},m}_{j_1^{'},m_1^{'},j_2^{'},m-m_1^{'}}\sum_{m_1^{''}=-j_1^{''}}^{+j_1^{''}} C^{j^{''},m}_{j_1^{''},m_1^{''},j_2^{''},m-m_1^{''}}$$

$$\times\sum_{\lambda_1\mu_1\lambda_2\lambda} \upsilon_{\lambda_1\mu_1\lambda_2\lambda}(R)\sqrt{\frac{2\lambda_1+1}{4\pi}}\sum_{\eta=-\min(\lambda_1,\lambda_2)}^{+\min(\lambda_1,\lambda_2)} C^{\lambda,0}_{\lambda_1,\eta,\lambda_2,-\eta}\sqrt{\frac{\left(2j_2^{'}+1\right)\left(2\lambda_2+1\right)}{4\pi\left(2j_2^{''}+1\right)}}C^{j_2^{''},0}_{j_2^{'},0,\lambda_2 0}C^{j_2^{''},m-m_1^{''}}_{j_2^{'},m-m_1^{'},\lambda_2-\eta}$$

$$\times\frac{8\pi^2}{2j_1^{''}+1}C^{j_1^{''},m_1^{''}}_{j_1^{'},m_1^{'},\lambda_1,\eta}\begin{bmatrix} \left(C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{'}\left(C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{'}\epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right) \end{bmatrix}$$

On further simplification we obtain,

$$M^{n''}_{n'} = \sqrt{\frac{2j_1^{'}+1}{2j_1^{''}+1}}\sqrt{\frac{2j_2^{'}+1}{2j_2^{''}+1}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{'},0}\right)2\left(1+\delta_{k_1^{''},0}\right)}}\sum_{\lambda_1\mu_1\lambda_2\lambda}\upsilon_{\lambda_1\mu_1\lambda_2\lambda}(R)\sqrt{\frac{2\lambda_1+1}{4\pi}}\sqrt{\frac{2\lambda_2+1}{4\pi}}$$

$$\times C^{j_2^{''},0}_{j_2^{'},0,\lambda_2 0}\sum_{m_1^{'}=-j_1^{'}}^{+j_1^{'}} C^{j^{'},m}_{j_1^{'},m_1^{'},j_2^{'},m-m_1^{'}}\sum_{m_1^{''}=-j_1^{''}}^{+j_1^{''}} C^{j^{''},m}_{j_1^{''},m_1^{''},j_2^{''},m-m_1^{''}}\sum_{\eta=-\min(\lambda_1,\lambda_2)}^{+\min(\lambda_1,\lambda_2)} C^{\lambda,0}_{\lambda_1,\eta,\lambda_2,-\eta}C^{j_2^{''},m-m_1^{''}}_{j_2^{'},m-m_1^{'},\lambda_2-\eta}C^{j_1^{''},m_1^{''}}_{j_1^{'},m_1^{'},\lambda_1,\eta}$$

$$\times\begin{bmatrix} \left(C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{'}\left(C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\ +\ \epsilon^{'}\epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda}C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right) \end{bmatrix}$$

In general, Clebsch-Gordan coefficients are non-zero only if $m = m_1 + m_2$ and $|j_1 - j_2| \le j \le j_1 + j_2$. Incorporating these properties of CG coefficients [1] we obtain the final state-to-state transition matrix element as follows:

$$
M^{n''}_{n'} = \sqrt{\frac{2j_1^{'}+1}{2j_1^{''}+1}}\sqrt{\frac{2j_2^{'}+1}{2j_2^{''}+1}}\sqrt{\frac{1}{2\left(1+\delta_{k_1^{'},0}\right)2\left(1+\delta_{k_1^{''},0}\right)}}\sum_{\lambda_1\mu_1\lambda_2\lambda} v_{\lambda_1\mu_1\lambda_2\lambda}(R)\sqrt{\frac{2\lambda_1+1}{4\pi}}
$$

$$
\times\sqrt{\frac{2\lambda_2+1}{4\pi}}\, C^{j_2^{''},0}_{j_2^{'},0,\,\lambda_2 0}\sum_{m_1^{'}=-j_1^{'}}^{+j_1^{'}} C^{j^{'},m}_{j_1^{'},m_1^{'},\,j_2^{'},m-m_1^{'}}\sum_{\eta=-\min(\lambda_1,\lambda_2)}^{+\min(\lambda_1,\lambda_2)} C^{j^{''},m}_{j_1^{''},m_1^{'}-\eta,\;j_2^{''},m-(m_1^{'}-\eta)}\, C^{\lambda,0}_{\lambda_1,\eta,\,\lambda_2,-\eta}\, C^{j_1^{''},m_1^{'}}_{j_1^{'},\,m_1^{'}-\eta,\,\lambda_1,\eta}
$$

$$
\times C^{j_2^{''},m-m_1^{'}}_{j_2^{'},\;m-\left(m_1^{'}-\eta\right),\,\lambda_2,-\eta}
\begin{bmatrix}
\left(C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda} C^{j_1^{''},k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\
+\;\epsilon^{'}\left(C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda} C^{j_1^{''},k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right) \\
+\;\epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda} C^{j_1^{''},-k_1^{''}}_{j_1^{'},k_1^{'},\lambda_1,-\mu_1}\right) \\
+\;\epsilon^{'}\epsilon^{''}\left(C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,\mu_1} + (-1)^{\lambda_1+\mu_1+\lambda_2+\lambda} C^{j_1^{''},-k_1^{''}}_{j_1^{'},-k_1^{'},\lambda_1,-\mu_1}\right)
\end{bmatrix}
$$

2. Additional figures for publication

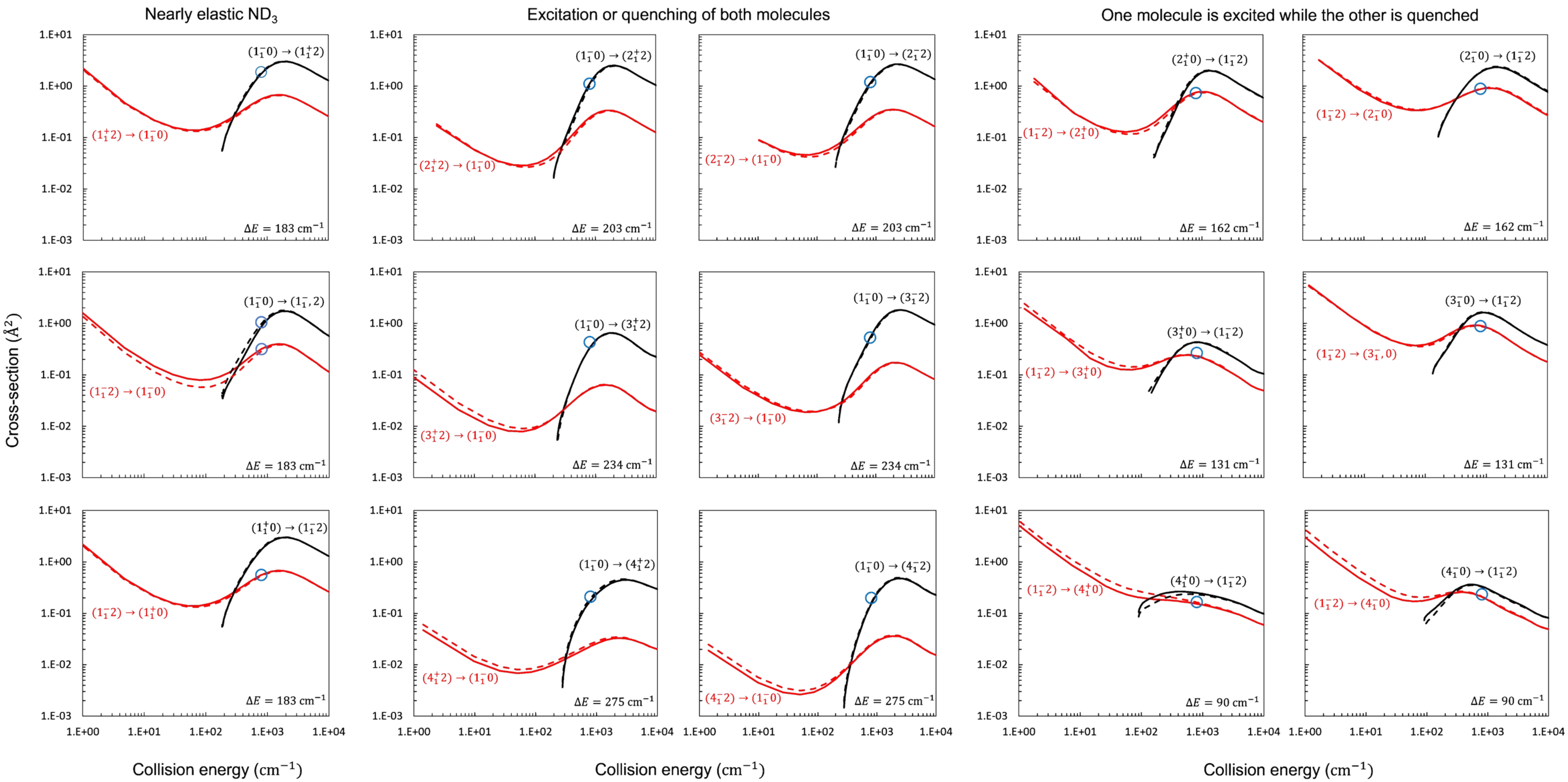

Figure S1: The test of microscopic reversibility for transitions between several rotational states of $ND_3 + D_2$ system, labeled as ($j_{1\,k}^{\,\pm} j_2$). Cross sections are plotted as a function of collision energy. The data obtained by “direct” MQCT calculations are shown by solid lines, whereas dashed lines represent the results of "reverse" calculations. Red color is used for quenching processes, black color is for excitation processes. Blue symbol indicates full-quantum results of Ref. [2].

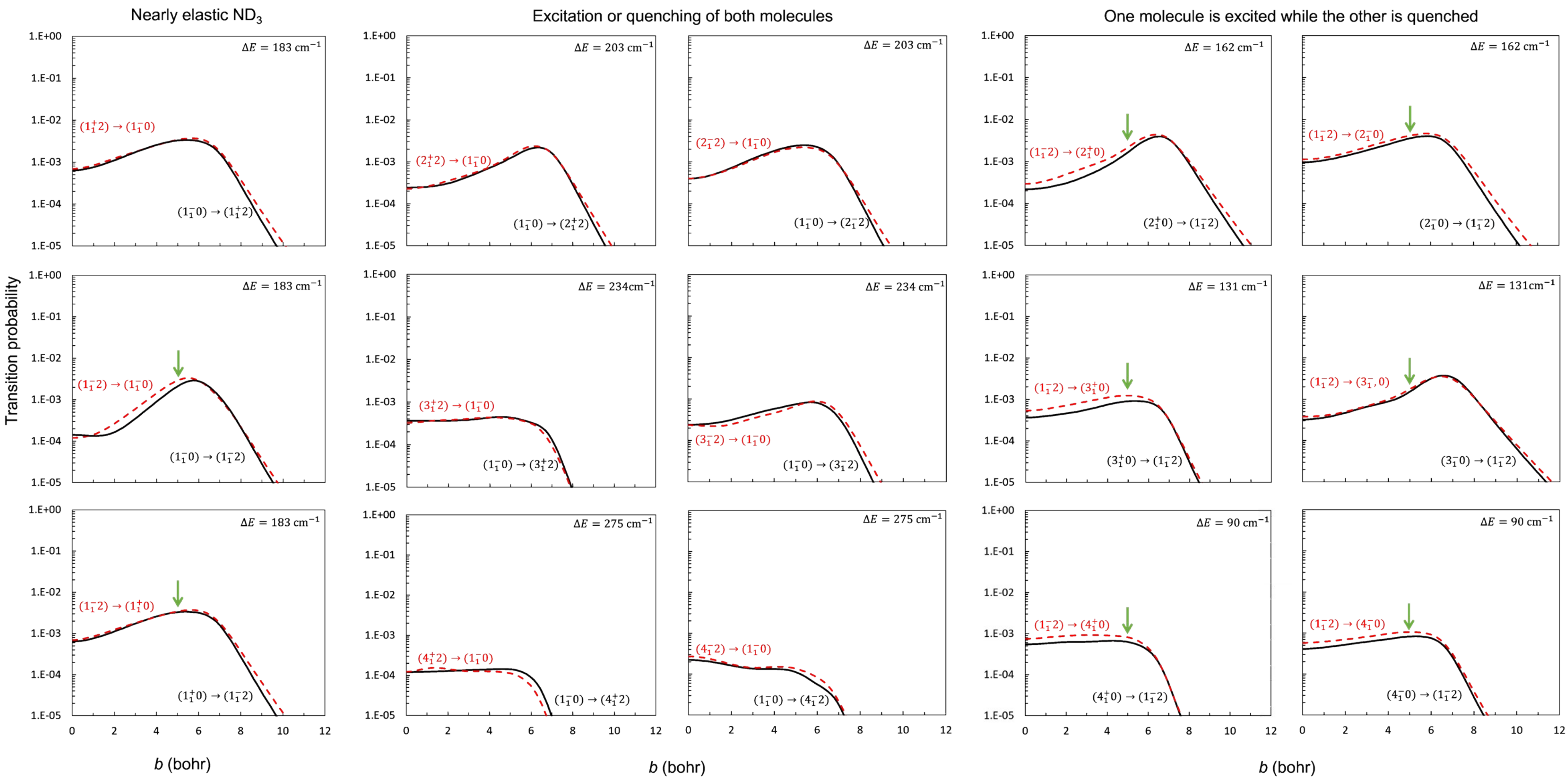

Figure S2: Opacity functions for several transitions between the rotational states of ND_3 + D_2 system, labeled as $(j_1 {}^{\pm}_{k} j_2)$. Transition probabilities are plotted as a function of collision impact parameter. Collision energy is 800 cm^{-1}. Red color is used for quenching processes, black color is for excitation processes. The value of energy difference is given for each transition. Green arrows indicate the value of impact parameter chosen for time-dependent analysis in Fig. 4 of the main text.

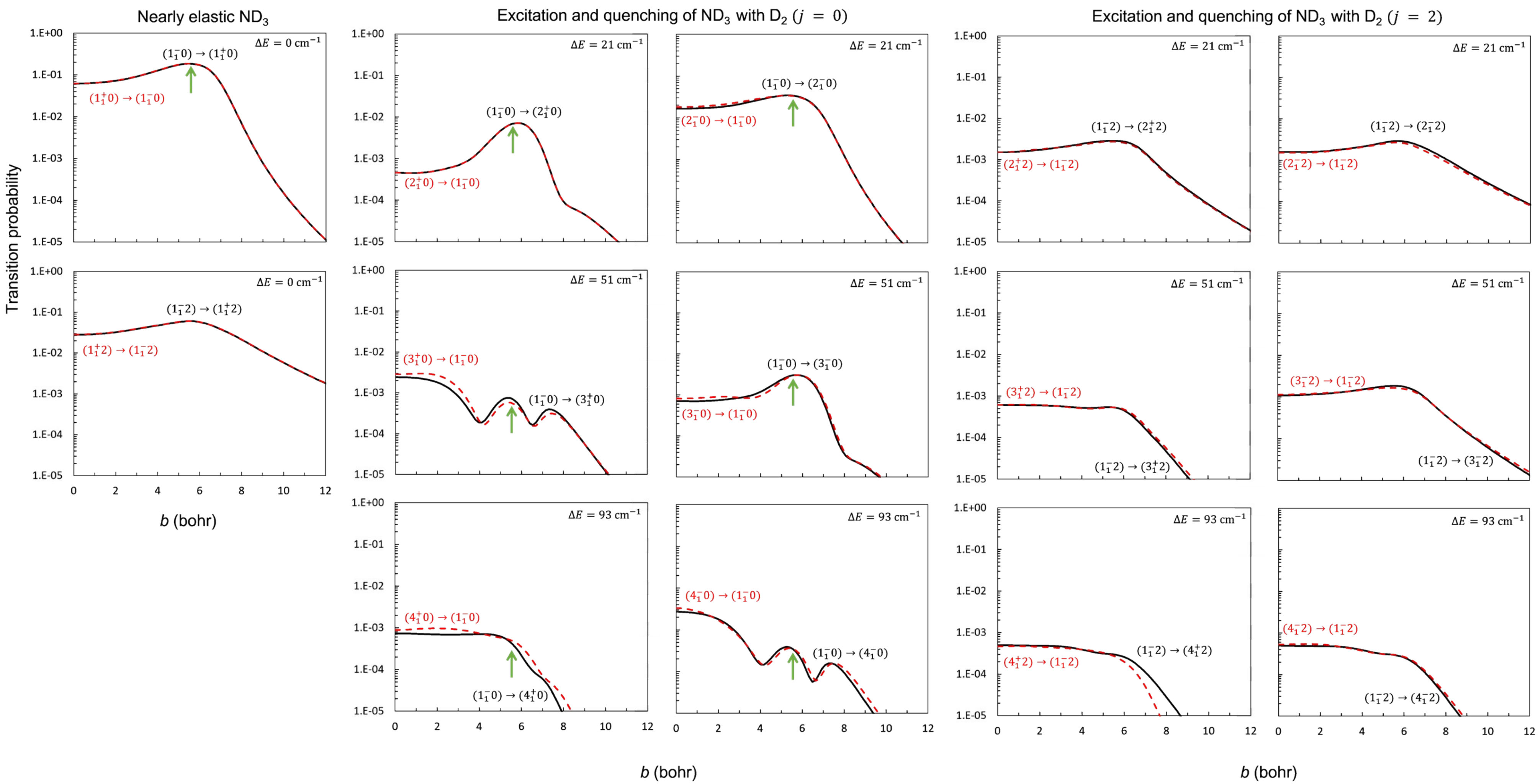

Figure S3: Opacity functions for several transitions between the rotational states of ND_3 + D_2 system, labeled as ($j_{1}{}_{k}^{\pm} j_2$) with D_2 (j_2) remaining in its initial state ($j_2 = 0$ or $j_2 = 2$). Transition probabilities are plotted as a function of collision impact parameter. Collision energy is 800 cm^{-1}. Red color is used for quenching processes, black color is for excitation processes. The value of energy difference is given for each transition. Green arrows indicate the value of impact parameter chosen for time-dependent analysis in Fig. 3 of the main text.

Table S1: Assignments of total (j,m)-components for all transitions discussed in this work in terms of potential coupling and Coriolis coupling. PD is for potential-driven transitions indicated by ✓ mark. If potential coupling is zero (× mark) the transition is driven only by Coriolis coupling. The fraction of Coriolis-driven components is indicated for each transition by red numbers.

Transition	j	m	PD
$(1_1^+0) \rightarrow (1_1^-2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (1_1^-0)$ 1/2	1	0	×
	1	1	✓
$(1_1^-0) \rightarrow (1_1^+0)$ 1/2	1	0	×
	1	1	✓
$\rightarrow (2_1^+0)$ 1/2	1	0	×
	1	1	✓
$\rightarrow (2_1^-0)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (3_1^+0)$ 1/2	1	0	×
	1	1	✓
$\rightarrow (3_1^-0)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (4_1^+0)$ 1/2	1	0	×
	1	1	✓
$\rightarrow (4_1^-0)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (1_1^+2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (1_1^-2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (2_1^+2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (2_1^-2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (3_1^+2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (3_1^-2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (4_1^+2)$ 0/2	1	0	✓
	1	1	✓
$\rightarrow (4_1^-2)$ 0/2	1	0	✓
	1	1	✓
$(1_1^+2) \rightarrow (1_1^-0)$ 5/9	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	×
	3	0	×
	3	1	✓
	3	2	×
	3	3	×
$\rightarrow (1_1^-2)$ 0/9	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓

Transition	j	m	PD
$(1_1^-2) \rightarrow (1_1^+0)$ 5/9	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	×
	3	0	×
	3	1	✓
	3	2	×
	3	3	×
$\rightarrow (1_1^-0)$ 4/9	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	×
	3	0	✓
	3	1	✓
	3	2	×
	3	3	×
$\rightarrow (2_1^+0)$ 3/9	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	×
	3	1	✓
	3	2	✓
	3	3	×
$\rightarrow (2_1^-0)$ 2/9	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	×
$\rightarrow (3_1^+0)$ 2/9	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	×
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (3_1^-0)$ 1/9	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (4_1^+0)$ 2/9	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	×
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (4_1^-0)$ 1/9	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓

Transition	j	m	PD
$(1_1^-2) \rightarrow (1_1^+2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (2_1^+2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (2_1^-2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (3_1^+2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (3_1^-2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (4_1^+2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$\rightarrow (4_1^-2)$ 0/9	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓

Transition	j	m	PD
$(2_1^+0) \rightarrow (1_1^-0)$ 2/3	2	0	×
	2	1	✓
	2	2	×
$\rightarrow (1_1^-2)$ 0/3	2	0	✓
	2	1	✓
	2	2	✓
$(2_1^-0) \rightarrow (1_1^-0)$ 1/3	2	0	✓
	2	1	✓
	2	2	×
$\rightarrow (1_1^-2)$ 0/3	2	0	✓
	2	1	✓
	2	2	✓
$(3_1^+0) \rightarrow (1_1^-0)$ 3/4	3	0	×
	3	1	✓
	3	2	×
	3	3	×
$\rightarrow (1_1^-2)$ 0/4	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$(3_1^-0) \rightarrow (1_1^-0)$ 2/4	3	0	✓
	3	1	✓
	3	2	×
	3	3	×
$\rightarrow (1_1^-2)$ 0/4	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
$(4_1^+0) \rightarrow (1_1^-0)$ 4/5	4	0	×
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
$\rightarrow (1_1^-2)$ 1/5	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
$(4_1^-0) \rightarrow (1_1^-0)$ 3/5	4	0	✓
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
$\rightarrow (1_1^-2)$ 1/5	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×

Table S1: *Continued*

Transition	j	m	PD
$(2_1^+2) \rightarrow (1_1^-0)$ 9/15	0	0	×
	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	×
	3	0	✓
	3	1	✓
	3	2	×
	3	3	×
	4	0	×
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
$\rightarrow (1_1^-2)$ 1/15	0	0	✓
	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
$(2_1^-2) \rightarrow (1_1^-0)$ 8/15	0	0	✓
	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	×
	3	0	×
	3	1	✓
	3	2	×
	3	3	×
	4	0	✓
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
$\rightarrow (1_1^-2)$ 1/15	0	0	✓
	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×

Transition	j	m	PD
$(3_1^+2) \rightarrow (1_1^-0)$ 13/20	1	0	×
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	×
	3	0	×
	3	1	✓
	3	2	×
	3	3	×
	4	0	✓
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
	5	0	×
	5	1	✓
	5	2	×
	5	3	×
	5	4	×
	5	5	×
$\rightarrow (1_1^-2)$ 3/20	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
	5	0	✓
	5	1	✓
	5	2	✓
	5	3	✓
	5	4	×
	5	5	×

Transition	j	m	PD
$(3_1^-2) \rightarrow (1_1^-0)$ 12/20	1	0	✓
	1	1	✓
	2	0	×
	2	1	✓
	2	2	×
	3	0	✓
	3	1	✓
	3	2	×
	3	3	×
	4	0	×
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
	5	0	✓
	5	1	✓
	5	2	×
	5	3	×
	5	4	×
	5	5	×
$\rightarrow (1_1^-2)$ 3/20	1	0	✓
	1	1	✓
	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
	5	0	✓
	5	1	✓
	5	2	✓
	5	3	✓
	5	4	×
	5	5	×

Transition	j	m	PD
$(4_1^+2) \rightarrow (1_1^-0)$ 18/20	2	0	×
	2	1	✓
	2	2	×
	3	0	✓
	3	1	✓
	3	2	×
	3	3	×
	4	0	×
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
	5	0	✓
	5	1	✓
	5	2	×
	5	3	×
	5	4	×
	5	5	×
	6	0	×
	6	1	✓
	6	2	×
	6	3	×
	6	4	×
	6	5	×
	6	6	×
$\rightarrow (1_1^-2)$ 6/25	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
	5	0	✓
	5	1	✓
	5	2	✓
	5	3	✓
	5	4	×
	5	5	×
	6	0	✓
	6	1	✓
	6	2	✓
	6	3	✓
	6	4	×
	6	5	×
	6	6	×

Transition	j	m	PD
$(4_1^-2) \rightarrow (1_1^-0)$ 17/20	2	0	✓
	2	1	✓
	2	2	×
	3	0	×
	3	1	✓
	3	2	×
	3	3	×
	4	0	✓
	4	1	✓
	4	2	×
	4	3	×
	4	4	×
	5	0	×
	5	1	✓
	5	2	×
	5	3	×
	5	4	×
	5	5	×
	6	0	✓
	6	1	✓
	6	2	×
	6	3	×
	6	4	×
	6	5	×
	6	6	×
$\rightarrow (1_1^-2)$ 6/25	2	0	✓
	2	1	✓
	2	2	✓
	3	0	✓
	3	1	✓
	3	2	✓
	3	3	✓
	4	0	✓
	4	1	✓
	4	2	✓
	4	3	✓
	4	4	×
	5	0	✓
	5	1	✓
	5	2	✓
	5	3	✓
	5	4	×
	5	5	×
	6	0	✓
	6	1	✓
	6	2	✓
	6	3	✓
	6	4	×
	6	5	×
	6	6	×

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