Supplemental Information for:

"On Mixed Quantum/Classical Theory for Rotationally Inelastic Scattering of Identical Collision Partners"

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In this work we did not pursue the goal of producing cross sections converged with respect to the size of rotational basis set. Therefore, small basis sets were used, sufficient to introduce all kinds of transitions as discussed in the paper: between pair \leftrightarrow pair, pair \leftrightarrow non-pair, non-pair \leftrightarrow non-pair states. These are summarized in Table S1. Other input parameters are given in Table S2.

Table S1: Rotational basis sets employed and the number of non-zero matrix elements for various collision partners considered in this work.

Collision partners	Maximum j ₁ , j ₂	Distinguishable			Indistinguishable		
		Channels	j₁j₂jm states	Matrix elements	Channels	$j_1 j_2 jm^{\pm}$ states [*]	Matrix elements [*]
$H_2 + H_2$	6 (even only)	16	784	20404	10	406, 378	5505, 4911
CO + CO	4	25	625	19395	15	325, 300	5249, 4626
$p-H_2O + p-H_2O$	2	25	361	9862	15	190, 171	2724, 2316

*First and second numbers correspond to positive and negative exchange parities, respectively.

Table S2: Other input parameters of MQCT calculations.

Collision	$R_{\min} - R_{\max}$ (Bohr)	Reduced mass (amu)	Max. impact parameter (Bohr)	Number of grid points			
partners				R	α_1, α_2	β_1, β_2	γ_1, γ_2
$H_2 + H_2$	2.0-50.0	1.0	20.0	100	0, 50	25, 25	0, 0
CO + CO	5.0-50.0	13.99746	20.0	76	0, 40	20, 20	0, 0
$H_2O + H_2O$	4.0-100.0	9.00764	30.0	100	30,30	15,15	30,30

Table S3: The list of transitions presented in this work for each of three systems studied. Transitions are grouped by their initial states, and each initial state is assigned a certain color. These colors are the same as colors of symbols in Fig. 4 of the main text and in Figs. S1-S3 below.

	pair ↔ pair (6 transitions)	pair ↔ r (18 tran	non-pair ↔ non-pair (6 transitions)		
H2	$(00) \rightarrow (22)$ $(00) \rightarrow (44)$	$(00) \rightarrow (20)$ $(00) \rightarrow (40)$ $(00) \rightarrow (42)$	$(20) \to (00)$ $(20) \to (22)$ $(20) \to (44)$	$(20) \rightarrow (40)$ $(20) \rightarrow (42)$	
$H_2 + H$	$(22) \rightarrow (00)$ $(22) \rightarrow (44)$	$(22) \rightarrow (20)$ $(22) \rightarrow (40)$ $(22) \rightarrow (42)$	$(40) \rightarrow (00)$ $(40) \rightarrow (22)$ $(40) \rightarrow (44)$	$(40) \rightarrow (20)$ $(40) \rightarrow (42)$	
	$(44) \rightarrow (00)$ $(44) \rightarrow (22)$	$(44) \rightarrow (20)$ $(44) \rightarrow (40)$ $(44) \rightarrow (42)$	$(42) \to (00)$ $(42) \to (22)$ $(42) \to (44)$	$(42) \rightarrow (20) (42) \rightarrow (40)$	
	pair ↔ pair (12 transitions)	pair ↔ r (45 tran	non-pair ↔ non-pair (27 transitions)		
	$(00) \rightarrow (11)$ $(00) \rightarrow (22)$ $(00) \rightarrow (33)$ $(00) \rightarrow (44)$	$\begin{array}{cccc} (00) \rightarrow (10) & (00) \rightarrow (32) \\ (00) \rightarrow (20) & (00) \rightarrow (40) \\ (00) \rightarrow (21) & (00) \rightarrow (41) \\ (00) \rightarrow (30) & (00) \rightarrow (42) \\ (00) \rightarrow (31) & (00) \rightarrow (43) \end{array}$	$(10) \rightarrow (00)$ $(10) \rightarrow (11)$ $(10) \rightarrow (22)$ $(10) \rightarrow (33)$ $(10) \rightarrow (44)$	$\begin{array}{cccc} (10) \rightarrow (20) \\ (10) \rightarrow (21) \\ (10) \rightarrow (30) \\ (10) \rightarrow (31) \\ (10) \rightarrow (32) \end{array} \begin{array}{c} (10) \rightarrow (40) \\ (10) \rightarrow (41) \\ (10) \rightarrow (42) \\ (10) \rightarrow (43) \end{array}$	
CO + CC	$(11) \to (00) (11) \to (22) (11) \to (33) (11) \to (44)$	$\begin{array}{ccc} (11) \rightarrow (10) & (11) \rightarrow (32) \\ (11) \rightarrow (20) & (11) \rightarrow (40) \\ (11) \rightarrow (21) & (11) \rightarrow (41) \\ (11) \rightarrow (30) & (11) \rightarrow (42) \\ (11) \rightarrow (31) & (11) \rightarrow (43) \end{array}$	$\begin{array}{c} (20) \to (00) \\ (20) \to (00) \\ (20) \to (22) \\ (20) \to (33) \\ (20) \to (44) \end{array}$	$\begin{array}{cccc} (20) \rightarrow (10) \\ (20) \rightarrow (21) \\ (20) \rightarrow (30) \\ (20) \rightarrow (31) \\ (20) \rightarrow (32) \end{array} \begin{array}{c} (20) \rightarrow (40) \\ (20) \rightarrow (41) \\ (20) \rightarrow (42) \\ (20) \rightarrow (43) \end{array}$	
	$(22) \to (00) (22) \to (11) (22) \to (33) (22) \to (44)$	$\begin{array}{cccc} (22) \rightarrow (10) & (22) \rightarrow (32) \\ (22) \rightarrow (20) & (22) \rightarrow (40) \\ (22) \rightarrow (21) & (22) \rightarrow (41) \\ (22) \rightarrow (30) & (22) \rightarrow (42) \\ (22) \rightarrow (31) & (22) \rightarrow (43) \end{array}$	$\begin{array}{c} (21) \to (00) \\ (21) \to (11) \\ (21) \to (22) \\ (21) \to (33) \\ (21) \to (44) \end{array}$	$\begin{array}{ccc} (21) \rightarrow (10) \\ (21) \rightarrow (20) \\ (21) \rightarrow (30) \\ (21) \rightarrow (31) \\ (21) \rightarrow (32) \end{array} \begin{array}{c} (21) \rightarrow (40) \\ (21) \rightarrow (41) \\ (21) \rightarrow (42) \\ (21) \rightarrow (43) \end{array}$	
	pair ↔ pair (9 transitions)	pair ↔ r (30 tran	non-pair ↔ non-pair (15 transitions)		
	$(0_{00}0_{00}) \rightarrow (1_{11}1_{11}) (0_{00}0_{00}) \rightarrow (2_{02}2_{02}) (0_{00}0_{00}) \rightarrow (2_{11}2_{11})$	$\begin{array}{c} (0_{00}0_{00}) \rightarrow (1_{11}0_{00}) \\ (0_{00}0_{00}) \rightarrow (2_{02}0_{00}) \\ (0_{00}0_{00}) \rightarrow (2_{02}1_{11}) \\ (0_{00}0_{00}) \rightarrow (2_{11}0_{00}) \\ (0_{00}0_{00}) \rightarrow (2_{11}1_{11}) \\ (0_{00}0_{00}) \rightarrow (2_{11}2_{02}) \end{array}$	$\begin{array}{c} (1_{11}0_{00}) \rightarrow (0_{00}0_{00}) \\ (1_{11}0_{00}) \rightarrow (1_{11}1_{11}) \\ (1_{11}0_{00}) \rightarrow (2_{02}2_{02}) \\ (1_{11}0_{00}) \rightarrow (2_{11}2_{11}) \end{array}$	$\begin{array}{c} (1_{11}0_{00}) \rightarrow (2_{02}0_{00}) \\ (1_{11}0_{00}) \rightarrow (2_{02}1_{11}) \\ (1_{11}0_{00}) \rightarrow (2_{11}0_{00}) \\ (1_{11}0_{00}) \rightarrow (2_{11}1_{11}) \\ (1_{11}0_{00}) \rightarrow (2_{11}2_{02}) \end{array}$	
$H_2O + H_2C$	$(1_{11}1_{11}) \rightarrow (0_{00}0_{00}) (1_{11}1_{11}) \rightarrow (2_{02}2_{02}) (1_{11}1_{11}) \rightarrow (2_{11}2_{11})$	$\begin{array}{c} (1_{11}1_{11}) \rightarrow (1_{11}0_{00}) \\ (1_{11}1_{11}) \rightarrow (2_{02}0_{00}) \\ (1_{11}1_{11}) \rightarrow (2_{02}1_{11}) \\ (1_{11}1_{11}) \rightarrow (2_{11}0_{00}) \\ (1_{11}1_{11}) \rightarrow (2_{11}1_{11}) \\ (1_{11}1_{11}) \rightarrow (2_{11}2_{02}) \end{array}$	$\begin{array}{c} (2_{02}0_{00}) \rightarrow (0_{00}0_{00}) \\ (2_{02}0_{00}) \rightarrow (1_{11}1_{11}) \\ (2_{02}0_{00}) \rightarrow (2_{02}2_{02}) \\ (2_{02}0_{00}) \rightarrow (2_{11}2_{11}) \end{array}$	$\begin{array}{c} (2_{02}0_{00}) \rightarrow (1_{11}0_{00}) \\ (2_{02}0_{00}) \rightarrow (2_{02}1_{11}) \\ (2_{02}0_{00}) \rightarrow (2_{11}0_{00}) \\ (2_{02}0_{00}) \rightarrow (2_{11}1_{11}) \\ (2_{02}0_{00}) \rightarrow (2_{11}2_{02}) \end{array}$	
	$(2_{02}2_{02}) \rightarrow (0_{00}0_{00}) (2_{02}2_{02}) \rightarrow (1_{11}1_{11}) (2_{02}2_{02}) \rightarrow (2_{11}2_{11})$	$\begin{array}{c} (2_{02}2_{02}) \rightarrow (1_{11}0_{00}) \\ (2_{02}2_{02}) \rightarrow (2_{02}0_{00}) \\ (2_{02}2_{02}) \rightarrow (2_{02}1_{11}) \\ (2_{02}2_{02}) \rightarrow (2_{11}0_{00}) \\ (2_{02}2_{02}) \rightarrow (2_{11}1_{11}) \\ (2_{02}2_{02}) \rightarrow (2_{11}2_{02}) \end{array}$	$\begin{array}{c} (2_{02}1_{11}) \rightarrow (0_{00}0_{00}) \\ (2_{02}1_{11}) \rightarrow (1_{11}1_{11}) \\ (2_{02}1_{11}) \rightarrow (2_{02}2_{02}) \\ (2_{02}1_{11}) \rightarrow (2_{11}2_{11}) \end{array}$	$\begin{array}{c} (2_{02}1_{11}) \rightarrow (1_{11}0_{00}) \\ (2_{02}1_{11}) \rightarrow (2_{02}0_{00}) \\ (2_{02}1_{11}) \rightarrow (2_{11}0_{00}) \\ (2_{02}1_{11}) \rightarrow (2_{11}1_{11}) \\ (2_{02}1_{11}) \rightarrow (2_{11}2_{02}) \end{array}$	



Figure S1: Ratios of inelastic cross sections for $H_2 + H_2$ obtained by treating collision partners either as indistinguishable or distinguishable in MQCT calculations at different collision energies. Top frames display the data for pair \leftrightarrow pair transition, middle frames for pair \leftrightarrow non-pair and lower frames for non-pair transitions. Results are obtained using three different versions of MQCT methods: CS-MQCT (left frames), CC-MQCT (middle frames) and AT-MQCT (right frames). Transitions are grouped by their initial states, and each initial state is assigned a certain color: blue for (00), orange for (22), dark green for (44), light blue for (20), violet for (40), light green for (42). The full list of presented transitions is given in Table S3.



Figure S2: Same as Fig. S1, but for CO + CO system. Transitions are grouped by their initial states, and each initial state is assigned a certain color: blue for (00), orange for (11), dark green for (22), light blue for (10), violet for (20), light green for (21). The full list of presented transitions is given in Table S3.



Figure S3: Same as in Fig. S1, but for p-H₂O + p-H₂O system. Transitions are grouped by their initial states, and each initial state is assigned a certain color: blue for ($0_{00}0_{00}$), orange for ($1_{11}1_{11}$), dark green for ($2_{02}2_{02}$), light blue for ($1_{11}0_{00}$), violet for ($2_{02}0_{00}$), light green for ($2_{02}1_{11}$). The full list of presented transitions is given in Table S3.