

## ABSTRACT

481780 ( ) ( & 76 , 1 & 2 // , 6 , 21 \$ / ( 1 ( 5 \* < 75 \$ 16 ) ( 5  
6 , 08 / \$ 7 ( ' 86 , MIXED QUANTUM/CLASSICAL THEORY

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Mixed quantum/classical theory was used to study collisional energy transfer between the rotational states of molecules with the focus on reproducing quantum effects related to this process. Namely, the rotational energy transfer in the  $\text{e-ND}$  system was studied to replicate quantum interference effect observed as oscillations of scattering cross section as a function of collision energy. Both MQCT code and the full-quantum code MOLSCAT were used for calculations, and results were in excellent agreement with the experiment and the full quantum infinite order sudden method from literature. The  $\text{CO} + \text{CO}$  system was used as a case study for diatom + diatom collisions. First, two CO molecules were created as distinguishable in order to compare results with available full quantum coupled states data. Excellent agreement between the two methods was achieved. It was found that for strong transitions with large cross sections, the results of MQCT are reliable, especially at higher collision energy. For weaker transitions with small cross sections, the results of MQCT are less reliable.