

Adiabatic model for cold molecule-molecule collisions : Application to rotational excitation of water colliding with para-Hydrogen molecule

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The Time Independent Quantum Method is the reference for the calculations of cold molecule-molecule collisions. This close-coupling (CC) approach is commonly used in the cold chemistry and molecular astrophysics communities. However, the numerical cost of the CC-method increases significantly with the size of the target molecule and some new methods should be investigated.

I will present the use of an adiabatic model (and its possible extension) in the context of the CC-method. I will present the results (inelastic cross sections and rate constants) for the water colliding with para-Hydrogen molecule. The internal rotational adiabatic decoupling scheme reduces dimensional dynamics from a 5D to a 3D problem and a good agreement is found between those two calculations. This adiabatic reduction of dimensionality seems very promising for scattering studies involving the excitation of a heavy target molecule by a light molecular projectile.