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Low-energy collisions between two indistinguishable tritium-bearing hydrogen molecules: HT+HT and DT+DT

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Tritium bearing hydrogen molecules are of a significant scientific interest, see Ref. [1] and, for instance, Tritium Laboratory Karlsruhe (TLK) reports at Karlsruhe Institute of Technology (Germany). In this work a quantum-mechanical close-coupling calculation is performed for elastic and inelastic 4-atomic collisions: $\mathrm{HT}(j_1)+\mathrm{HT}(j_2) \rightarrow \mathrm{HT}(j_1')+\mathrm{HT}(j_2')$ and $\mathrm{DT}(j_1)+\mathrm{DT}(j_2) \rightarrow \mathrm{DT}(j_1')+\mathrm{DT}(j_2')$. Here H is a hydrogen atom, D is deuterium, and T is tritium. Global six-dimensional symmetrical H_2-H_2 potential energy surfaces (PESs) [2,3] have been adopted and appropriately modified for current 4-atomic systems. Specifically, we changed the position of the center of mass in HT and DT. In this presentation a special attention will be given to different geometrical modifications of the multidimensional H_2-H_2 potentials, as in Ref.[4]. State-resolved integral cross sections $\sigma_{j_1 j_2 \rightarrow j_1' j_2'}(\varepsilon_{kin})$ for quantum-mechanical rotational transitions $j_1 j_2 \rightarrow j_1' j_2'$ in HT and DT molecules and corresponding state-resolved thermal rate coefficients $k_{j_1 j_2 \rightarrow j_1' j_2'}(T)$ have been computed. The relationship between the rate coefficient $k_{j_1 j_2 \rightarrow j_1' j_2'}(T)$ and the cross section $\sigma_{j_1 j_2 \rightarrow j_1' j_2'}(\varepsilon)$ can be obtained through the following weighted average: $k_{j_1 j_2 \rightarrow j_1' j_2'}(T) = \sqrt{\frac{8k_BT}{\pi\mu}} \frac{1}{(k_BT)^2} \int_{\varepsilon_s}^{\infty} e^{-\varepsilon/k_BT} \times \sigma_{j_1 j_2 \rightarrow j_1' j_2'}(\varepsilon)\varepsilon d\varepsilon$, where k_B is Boltzmann constant, μ is reduced mass of the molecule-molecule system and ε_s is the minimum kinetic energy for the levels j_1 and j_2 to become accessible. Additionally, for comparison purposes, H_2+H_2/HD calculations for a few selected rotational transitions have also been performed. These energy transfer collisions are of fundamental importance in astrophysics, see for example Refs.[5-7], papers [4] and Ref. [8]. The hydrogen molecules HT and DT are treated as rigid rotors in our calculations. A pronounced isotope effect is identified in the title collisions.

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