ROTATIONAL ENERGY TRANSFER IN o-/p-H_2+HD AT LOW TEMPERATURES

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Quantum-mechanical close-coupling calculations for rotational state resolved cross sections and thermal rate coefficients for the o-/p-H_2+HD collisions of astrophysical interest will be presented. Recently developed new global H_2-H_2 potential energy surface[a] has been appropriately adopted for H_2 + HD and applied. The low temperature limit of o-/p-H_2+HD is investigated, which is of significant astrophysical interest in regard to the cooling of primordial gas and the interstellar media. A test of convergence and the results for cross sections with the new potential[a] are obtained for a wide range of kinetic velocities including values down to $\sim$10 m/s. Sharp resonances have been reproduced in the cross sections of some transition states at very low energies.
Our results revealed[b], that for lower quantum transition states the new surface provides cross sections very close to those obtained in previous works, where the authors adopted some old potentials for H_2-H_2. However, for higher quantum states we found significant disagreements with previous results. Additionally, in our calculations new resonances are calculated in the 1300 ± 100 m/s region[b]. The value of the resonances are relatively large, and it may exert a strong influence on the cooling processes in primodial gas and interstellar media.

[a] A.I. Boothroyd, P. G. Martin, W. J. Keogh, M. J. Peterson, J. Chem. Phys., 116, 666 (2002).
[b] R.A. Sultanov, D. Guster, Chem. Phys. Lett. 436, 19 (2007).