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Nonrigidity effects in the He(1s2s)+H₂ collision pair MARIUSZ PAWLAK, PIOTR S. ZUCHOWSKI, PIOTR JANKOWSKI, Nicolaus Copernicus University in Torun, Poland, NIMROD MOISEYEV, Technion-Israel Institute of Technology, Haifa, Israel — Low-energy collisions exhibit the quantum nature of matter and physical phenomena. In our work, we show a crucial role of the flexibility of molecule in anisotropic atom–diatom collisions in sub-kelvin regime. We study Penning ionization reactions between excited helium atoms and ground state hydrogen molecules. Our results from state-of-the-art *ab initio* calculations are in excellent agreement with the recent experimental findings [Klein *et al.* Nature Phys. 13, 35–38 (2017)]. We reveal that the nonrigidity effect of H₂ on the reaction rate structure, not recognized in the previous study, is indispensable to correctly describe the observed resonances without a need for any empirical adjustment. We demonstrate that the approach beyond the widely used rigid-rotor approximation is required even when rigorous computations are carried out at the FCI level of theory.

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