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Near-thresholds inelastic collisions of water isotopes

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Water is the third most abundant molecule in the interstellar medium (ISM) and has ubiquitously been observed by ground- and space-based telescopes since its first detection in 1969 in the Orion nebula [1]. Thus water is a key molecule for the understanding of the energy balance and the physical-chemical processes that occur in these environments. Its principal collision partner obviously is H₂ because of its high abundance in ISM. Therefore, an accurate description of H₂O-H₂ collision dynamics is required at **low temperature/energy**, where the quantum nature of interaction may be revealed by the observation of **resonances** (Feshbach or shape/orbiting) [2].
The first rotational excitations of the water isotopologues by collisions with H₂ were observed in the near-cold regime in a crossed-molecular beam apparatus (CMB). The experimental scattering cross-sections were compared with the theoretical calculations performed on the potential energy surface of Valiron et al. [3], both at the state-to-state level and at low collision energy (near rotational thresholds) [4-6]. The different dynamical behaviors of H₂O, D₂O and HOD, colliding with *normal*- or *para*-H₂ will be presented.
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References
[1] E. F. van Dishoeck, E. Herbst, D. A. Neufeld, "Interstellar Water Chemistry: From Laboratory to Observations"Chem. Rev. 113, 9043-9085 (2013).
[2] Book: "Cold Chemistry: Molecular Scattering and reactivity Near Absolute Zero", Ed. O. Dulieu and A. Osterwalder, RSC (2017).
[3] P. Valiron et al., "R12-calibrated H₂O –H₂ interaction: Full dimensional and vibrationally averaged potential energy surfaces"J. Chem. Phys. 129, 134306 (2008).
[4] Bergeat A. et al., "Low-Energy Water–Hydrogen Inelastic Collisions"J. Phys. Chem. A 124, 259-264 (2020).
[5] Bergeat A. et al., "Probing Low-Energy Resonances in Water-Hydrogen Inelastic Collisions"Phys. Rev. Lett. 125, 143402(2020)
[6] Bergeat A. et al., Near-threshold and Resonance Effects in Rotationally Inelastic Scattering of D₂O with *normal*-H₂"Molecules 27, 7535(2022)

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