The smallest ice cube

Klavs Hansen
Center for Joint Quantum Studies and Department of Physics, School of Science, Tianjin University, China

Measured evaporative decay of mixed heavy and light water clusters show a remarkable scaling with the deuterium mole fraction above cluster size 8, including across the well-known shell closing at $N = 21$ [1], with values consistent with macroscopic surfaces. Helmholtz free energy differences of competing channels derived from these distributions [2] take the simplest possible form of a single energy parameter and the deuterium-protium mixing entropy. The results rule out any H-H interaction above the sub-meV scale. Comparison with similar experiments on partially deuterated ammonia clusters emphasize the special properties of water [3].

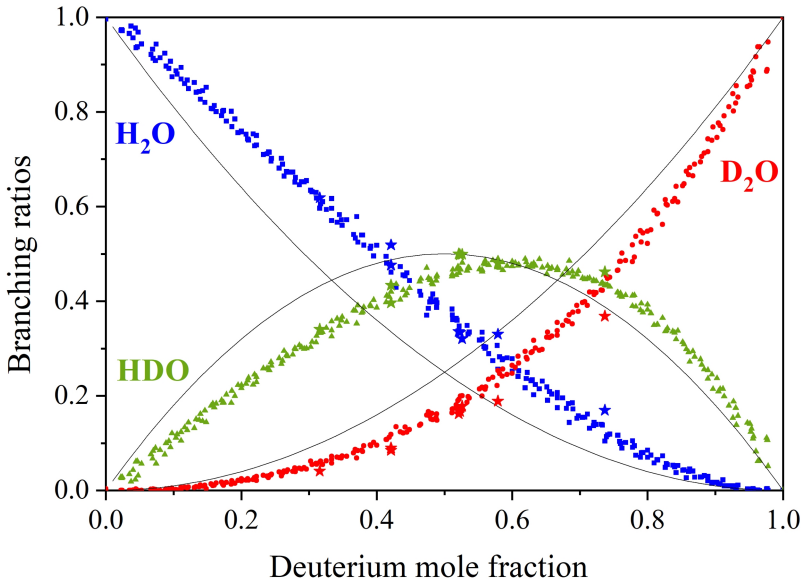

Fig.1 Evaporative branching ratios for water clusters $N = 9–14$ and N = 20–22. The lines are the calculated curves for a completely random distributions of deuterium and protium, and the points are the experimental values for H_2O (blue squares), HDO (olive triangles), and D_2O (red circles), all electrospray (room temperature) source data; stars are helium droplet (cryogenic source) measurements, color coded identically.

References

[1] Klavs Hansen, Kaveh Najafian, Bertil Dynefors, Mauritz J. Ryding, Einar Uggerud, Siegfried Kollotzek, Johannes Reichegger, Olga V. Lushchikova, and Paul Scheier "Bulk-Water Behavior of Water Clusters Studied by Isotope Effects", Phys. Rev. Lett. **136** (2026) 048001
[2] A.E.K. Sundéen, K. Støchkel, P. Hvelplund, S. Brøndsted Nielsen, B. Dynefors, and K. Hansen "Stabilities of protonated water-ammonia clusters" J. Chem. Phys. **148** (2018) 184306
[3] Klavs Hansen, Johannes Reichegger, Siegfried Kollotzek, Paul~Scheier *in preparation*