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Effect of hydrogen bond cooperativity on the phase behavior of water KEVIN STOKELY, Boston University Physics Department — Four scenarios have been proposed for the low–temperature phase behavior of liquid water, each predicting different thermodynamics. The physical mechanism which leads to each is debated. Moreover, it is still unclear which of the scenarios best describes water, as there is no definitive experimental test. Here we address both open issues by analyzing a microscopic cell model within a mean–field limit. We show that a common physical mechanism underlies each of the four scenarios, and that two key physical quantities determine which of the four scenarios describes water: (i) the strength of the directional component of the hydrogen bond and (ii) the strength of the cooperative component of the hydrogen bond. The four scenarios may be mapped in the space of these two quantities. Using estimates from experimental data for H bond properties, the model predicts that the low-temperature phase diagram of water exhibits a liquid–liquid critical point at positive pressure.

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