Supplementary Online Material:
The Distribution of Acceptor and Donor Hydrogen-Bonds in Bulk Liquid Water

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Tables for the joint distributions, $p_{ij}$, are given below for both AMOEBA and TIP3P water models at various temperatures for which water was simulated herein. These tables extend Table 1 in the text, which is limited to 300 K. These data are extracted from the coordinates of the classical trajectories, using the definition of a HB given in the text. From these data, the various distributions discussed in the text (overall/specific, unconditional/conditional) can be calculated by the equations provided in the Theory section.
Table 1. The joint donor (i)–acceptor (j) probabilities, \( p_{ij} \), calculated from AMOEBA and TIP3P trajectories at the indicated temperatures. \((-k)\) denotes \( \times 10^{-k} \).