Phase Transition in a Model of Y-shaped Molecules[1] DONOVAN
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— Increasing attention in statistical mechanics is being given to non-spherical
molecules, such as polypeptide chains and protein molecules. One example is pro-
vided by immunoglobulin, which has a "Y" shape. In this work, we determine the
phase diagram of "Y"-shaped molecules on a triangular lattice through Monte Carlo
Grand Canonical ensemble simulation, using histogram reweighting,multicanonical
sampling and finite size scaling. We show that (as expected) this model is a member
of the Ising universality class. For low temperatures, we implemented multicanonical
sampling to induce faster phase transitions in the simulation. By studying several
system sizes, we use finite size scaling to determine the two phase coexistence curve,
including the bulk critical temperature, critical chemical potential and critical den-
sity.

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