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Calculation of the configurational entropy for a binary Lennard-Jones fluid below the mode-coupling temperature using a hybrid Monte Carlo method ELIJAH FLENNER, GRZEGORZ SZAMEL, Dept. of Chemistry, Colorado State University — We developed a novel, hybrid Monte Carlo algorithm that combines configurational bias particle swaps with parallel tempering. We use this new method to simulate a standard model of a glass forming binary mixture above and below the so-called mode-coupling temperature, T_{MCT}. We find that an *ansatz* that was used previously to extrapolate thermodynamic quantities to temperatures below T_{MCT} breaks down in the vicinity of the mode-coupling temperature. Thus, previous estimates of the so-called Kauzmann temperature need to be reexamined. Also, we find that the Adam-Gibbs relations $D \propto \exp(-a/TS_c)$ and $\tau \propto \exp(b/TS_c)$, which connect the diffusion coefficient D and the relaxation time τ with the configurational entropy S_c, are valid for all temperatures for which the configurational and vibrational contributions to the free energy decouple.

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