High Precision Simulation Results for the Free Energy of Crystal from Acceptance Ratio Method and Expanded Ensemble Method

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Accurate values of the free energies of Lenard-Jones (LJ) crystal, cubic crystal of C60 and non-cubic crystal of C70 are obtained by using EE and BAR methods with Einstein molecule approach. Values for free energy of LJ crystal from BAR and EE methods give an order of magnitude higher accuracy than TI method as is seen from Table 1. Moreover, low-temperature solid-solid phase transition temperature of C70 crystals is determined from the free energy profiles with potential model of Sprik et al.[Phys. Rev. Lett. 69, 1660 (1992)]. This result which is found to be 180 K is consistent with the results of Sprik et al.'s molecular dynamics simulation. Through calculation of free energies of C70 crystal, we note particularly the importance of quantum correction for the indistinguishability of orientationally disordered crystals.