

MODIFICATION OF THE MAYER
SAMPLING METHOD FOR THE CALCULATION
OF HIGH-ORDER VIRIAL COEFFICIENTS

M. V. Ushcats

Admiral Makarov National University of Shipbuilding
(9, Stalingrad Heroes Str., Mykolaiv 54025, Ukraine;
e-mail: mykhailo.uscats@nuos.edu.ua)

S u m m a r y

A technique for the calculation of high-order virial coefficients, which combines the quadrature integration and the Mayer sampling Monte Carlo method (MSMC), is proposed. Unlike the original MSMC, this technique does not require to know the reference coefficients for the hard-sphere potential and can be used in a wide range of temperatures and for various interaction potentials. In addition, the proposed method has a higher accuracy at lower computational costs. It has been used to obtain some new data on the seventh virial coefficient of the Lennard-Jones (12-6) model.