Alignment of Buckingham Parameters to Generalized Lennard-Jones Potential Functions

Teik-Cheng Lim

School of Science and Technology, SIM University, 535A Clementi Road, S 599490, Republic of Singapore

Reprint requests to T.-C. L.; E-mail: alan_tc_lim@yahoo.com

Z. Naturforsch. **64a,** 200 – 204 (2009); received July 8, 2008 / revised August 21, 2008

The Lennard-Jones(12-6) and the Exponential-6 potential functions are commonly used in computational softwares for describing the van der Waals interaction energy. Some softwares allow switching between these two potentials under prescribed condition(s) that attempt to connect the parameter relationship between the two functions. Here we propose a technique by which the parameter relationship between both potentials is extracted by simultaneously imposing an equal force constant at the well depth's minimum and an equal mean interatomic energy from the point of equilibrium to the point of total separation. The former imposition induces good agreement for the interatomic compression and a small change in the interatomic distance near the equilibrium while the latter enables good agreement for large interatomic separation. The excellent agreement exhibited by the plots validates the technique of combined criteria proposed herein.

Key words: Parameter Conversion; Potential Function; van der Waals.
PACS numbers: 33.15.Dj, 33.15.Fm, 34.20.Cf