

# The Relationship between Lennard-Jones (12-6) and Morse Potential Functions

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Z. Naturforsch. **58a**, 615 – 617 (2003); received January 23, 2003

The most commonly used potentials for van der Waals interactions are the Exponential-6 and the Lennard-Jones (12-6) potential. In this paper a correlation between them is described. The Morse function, which is normally applied for quantifying 2-body interactions, has been adopted in one software. This paper deals with the validity of the Morse function for non-bonded interactions by means of obtaining a relationship between the Morse and the Lennard-Jones (12-6) potential functions. An approximate and an exact mathematical relationship is demonstrated to exist between these two potentials.

*Key words:* Lennard-Jones; Mathematical Relationship; Morse; Potential Functions; van der Waals.