INCORPORATING DAMPING FUNCTIONS INTO THE MORSE/LONG-RANGE POTENTIAL FUNCTION FORM IMPROVES BOTH LONG-RANGE AND VERY SHORT-RANGE BEHAVIOUR

ROBERT J. LE ROY, CARL HAUGEN and JASON TAO , *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.*

In recent years it has become increasingly common to analyze diatomic molecule spectroscopic data by using fully quantum mechanical direct potential fits (DPFs) to determine the potential energy function(s) of the state(s) in question. However, the efficacy of this approach is strongly dependent on the quality of the analytic model used for the potential function. The best global analytic model introduced to date is (arguably) the 'Morse/Long-Range' (MLR) function,[a] which provides particularly compact flexible functions which explicitly incorporate correct long-range. To date, applications of this form have mainly used a simple sum of inverse-power terms to represent the long-range behaviour. However, that neglects the fact that dispersion and other inverse-power terms change character at shorter distances where the electron distributions on the two moities begin to overlap.[b] With illustrative applications to MgH, Ca_2 and NaRb, we show that in addition to yielding more physically realistic long-range behaviour, including appropriately designed 'damping functions' with these inverse-power terms also gives potential functions with more realistic short-range behaviour.

[a] R.J. Le Roy and R.D.E. Henderson, Mol. Phys. **105**, 663 (2007); R.J. Le Roy *et al.*, *J. Chem. Phys.* **131** 204309 (2009).

[b] H. Kreek and W.J. Meath, *J. Chem. Phys.* **50**, 2289 (1969); H. Kreek, Y.H. Pan and W.J. Meath, *Mol. Phys.* **19**, 513 (1970)