MERGING OF THE SPLINE-POINTWISE AND MORSE/LONG-RANGE POTENTIAL FUNCTION FORMS FOR DIRECT-POTENTIAL-FIT DATA ANALYSES

JASON TAO, ROBERT J. LE ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*; ASEN PASHOV, *Department of Physics, Sofia University, 5 James Bourcheier blvd, 1164 Sofia, Bulgaria*.

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 two best models introduced to date are the 'Morse/Long-Range' (MLR) function[a] which provides particularly compact, accurate and flexible functions which explicitly incorporate correct long-range and sensible short-range behaviour, and the 'Spline Point-wise Potential' (SPP) form which is particularly successful for treating states with irregularly shaped potentials with a double-minimum or a 'shelf'.[b] The present work shows that a merging of these two forms effected by representing the exponent coefficient function of the MLR model by a spline passing through a compact mesh of values yields most of the advantages of both approaches. Preliminary illustrative applications to the ground states of Ca_2 and NaRb will be presented.

[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] A. Pashov, W. Jastrzębski and P. Kowalczyk, *Comp. Phys. Comm.* **128**, 622 (2000); *ibid, J. Mol. Spectrosc.* **203**, 264 (2000).