A GLOBAL MODEL FOR LONG-RANGE INTERACTION 'DAMPING FUNCTIONS'

PHILIP THOMAS MYATT, FREDERICK R. W. McCOURT, ROBERT J. LE ROY, *Department of Chemistry, University of Waterloo, Waterloo, ON, Canada*.

In recent years, 'damping functions', which characterize the weakening of inverse-power-sum long-range interatomic interaction energies with increasing electron overlap, have become an increasing important component of models for diatomic molecule interaction potentials.[a] However, a key feature of models for damping functions, their portability, has received little scrutiny. The present work set out to examine all available *ab initio* induction and dispersion damping function data[b] and to attempt to devise a 'global' scheme for diatomic molecule damping functions. It appears that while neutral (H, He, Li, and Ne, homonuclear and mixed) and anion ($H^-$ with H, He and Li) species obey (approximately) one common rule, proton plus neutral ($H^+$ with H, He and Li) and non-proton-cation plus neutral systems ($He^+$ and $Li^+$ with H, He and Li), must each be treated separately. However, for all three cases, a version of the Douketis-Scoles-Thakkar[c] $(\text{ionization potential})^{\text{power}}$ factor is a key scaling parameter.

---

[a] R.J. Le Roy, C. C. Haugen, J. Tao and Hui Li, *Mol. Phys.* **109**,435 (2011).

[b] P.J. Knowles and W.J. Meath,*J. Mol. Phys.* **60**, 1143 (1987); R.J. Wheatley and W.J. Meath,*J. Mol. Phys.* **80**, 25 (1993); R.J. Wheatley and W.J. Meath *J. Chem. Phys.* **179**, 341 (1994); R.J. Wheatley and W.J. Meath,*J. Chem. Phys.* **203**, 209 (1996).

[c] C. Douketis,G. Scoles, S. Marchetti, M. Zen and A. J. Thakkar, *J. Chem. Phys.* **76**, 3057 (1982).