METHODS OF SCALING QUANTUM MECHANICAL MOLECULAR FORCE FIELDS

YURII N. PANCHENKO, *Laboratory of Molecular Spectroscopy, Division of Physical Chemistry, Department of Chemistry, M. V. Lomonosov Moscow State University, 119899 Moscow, Vorobiovy gory, Russian Federation, C. I. S.*

A comparative analysis of various methods of empirical scaling of the quantum mechanical harmonic molecular force fields has been performed. The Pulay method of scaling is stressed to be applicable most successfully in the case where the quantum mechanical force field is determined close to the Hartree-Fock limit. This makes it possible to carry out correction of this force field with maximal retention of the peculiarities inherent in the the molecule under investigation.

The solution of the inverse vibrational problem using quantum mechanical force field as a starting one may be considered to be the limiting case of scaling with maximum number of scale factors. Such approach corresponds to the traditional philosophy that searching force field should be closest to the starting one[a]. On the contrary, the main physical criterion used in the Pulay scaling procedure is closeness of the vibrational modes determined from the scaled force field to the vibrational modes obtained from the starting quantum mechanical force field[b].

---

[a] A. G. Yagola, I. V. Kochikov, G. M. Kuramshina and Yu. A. Pentin. "Inverse Problems of Vibrational Spectroscopy". VSP, Utrecht, The Netherlands, 1999. Chapter 11, p. 259.

[b] Yu. N. Panchenko, *J. Mol. Struct.* **410-411**, 327 (1997).