

## VIBRATIONAL ANHARMONICITY AND SCALING THE QUANTUM MECHANICAL MOLECULAR FORCE FIELD

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The interrelationship between the scale factors obtained using Pulay's method <sup>a</sup> from the anharmonic and the harmonized vibrational frequencies of a light molecule and its heavy analogue is considered in terms of a Morse potential. The determination of the scale factors from the vibrational frequencies of a light molecule is shown to result in smaller deviations of the calculated and experimental vibrational frequencies of its heavy analogue than those of the reverse procedure. In this context the extent to which Dennison's rule <sup>b</sup> is satisfied is also discussed.

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<sup>a</sup>Yu. N. Panchenko, P. Pulay and F. Török, *J. Mol. Struct.* **34**, 283 (1976); V. I. Pupyshev, Yu. N. Panchenko, Ch. W. Bock and G. Pongor, *J. Chem. Phys.* **94**, 1247 (1991); Yu. N. Panchenko, G. R. De Maré and V. I. Pupyshev, *J. Phys. Chem.* **99**, 17544 (1995); Yu. N. Panchenko, *Moscow Univ. Chem. Bull.* **51**(5), 23 (1996).

<sup>b</sup>D. M. Dennison, *Rev. Mod. Phys.* **12**, 175 (1940); G. E. Hansen and D. M. Dennison, *J. Chem. Phys.* **20**, 313 (1952).