

## TRANSFERABILITY OF SCALE FACTORS VERSUS TRANSFERABILITY OF FORCE CONSTANTS

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In the techniques for solving the inverse vibrational problem on the basis of quantum-mechanical force fields, it is assumed that *the force constants are the same* for quasi-equivalent coordinates in similar structural moieties of related molecules<sup>a</sup>. Clearly, this approach ignores characteristics of the force field of each particular molecule. Indeed, this concept implies that all responsibility for possible shifts of frequencies and other spectral features of related molecules (to which the force constants are transferred) lies with changes in the inverse kinetic energy matrix.

With scaling of quantum-mechanical force fields, *the relative errors* introduced during quantum-mechanical calculations of force constants at a certain theoretical level are assumed to be approximately *the same* for quasi-equivalent coordinates in similar structural fragments of related molecules. This assumption imposes less stringent constraints than the assumption of transferability of force constants in series of related molecules<sup>b</sup>.

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<sup>a</sup>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.

<sup>b</sup>Yu. N. Panchenko, *J. Struct. Chem.* **40**, 548 (1999) (Russian pagination).