

## TRANSFERABILITY OF PULAY'S SCALE FACTORS IN THE IVa GROUP OF THE MENDELEYEV PERIODIC SYSTEM

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*Ab initio* quantum mechanical calculations were performed for structures and force fields (HF/6-31G\*//HF/6-31G\*<sup>a</sup>) of 3,3-dimethylbutene-1, cyclopropene, 1-methylcyclopropene, and 1-trimethylsilyl-, 1,2-bis(trimethylsilyl)-, 1-trimethylgermyl-, 1,2-bis(trimethylgermyl)-, 1-trimethylstannyl-, and 1,2-bis(trimethylstannyl)-3,3-dimethylcyclopropene. Scale factors for correction of the quantum mechanical force fields of cyclopropene, 1-methylcyclopropene, and 3,3-dimethylbutene-1 were determined using Pulay's scaling method.<sup>b</sup> Only the experimental vibrational frequencies of the light isotopomers of these molecules were used in the scaling procedure. The set of scale factors obtained was transferred to the quantum mechanical force fields of all the other molecules mentioned above. The vibrational problems for these molecules were solved. Complete vibrational analyses were carried out for the whole set of these related compounds. Transferability of scale factors for series of related compounds of cyclopropene with heteroatoms from the IVa group of the Mendeleev Periodic System of chemical elements was demonstrated.

<sup>a</sup>P. C. Hariharan and J. A. Pople, *Chem. Phys. Lett.* **16**, 217 (1972).

<sup>b</sup>Yu. N. Panchenko, P. Pulay and F. Török, *J. Mol. Structure* **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).