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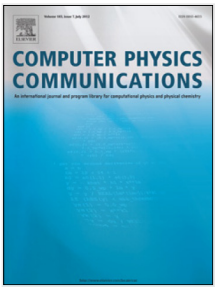

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Computational Thermochemistry: Automated Generation of Scale Factors for Vibrational Frequencies Calculated by Electronic Structure Model Chemistries

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Abstract. We present a Python program, Freqscale, for calculating the optimal scale factors for calculating harmonic vibrational frequencies, fundamental vibrational frequencies, and zero-point vibrational energies from electronic structure calculations. The program utilizes a previously published scale factor optimization model [I. M. Alecu, J. Zheng, Y. Zhao, D. G. Truhlar, J. Chem. Theory Comput. 6 (2010) 2872] to efficiently obtain all three scale factors from a set of computed vibrational harmonic frequencies. In order to obtain the three scale factors, the user only needs to provide zero point energies of 15 or 6 selected molecules. If the user has access to the *Gaussian09* or *Gaussian03* program, we provide the option for the user to run the program by entering the keywords for a certain method and basis set in the *Gaussian09* or *Gaussian03* program. Four other Python programs, input.py, input6, pbs.py, and pbs6.py are also provided for generating *Gaussian 09* or *Gaussian 03* input and pbs files. The program can also be used with data from any other electronic structure package. A manual of how to use this program is included in the code package.

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