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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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