

USER MANUAL  
FOR  
FREQSCALE

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

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## Contents

Executive Summary	2
Background Reading and Recommended Citations	2
Usage	2
Package	2
Platform	2
Installation	3
Examples of running the Program	3
Input and Output for Test run 1	4
Input and Output for Test run 2	6
Input and Output for Test run 3	7
Input and Output for Test run 4	9
Input and Output for Test run 5	10
Input and Output for Test run 6	12
Input and Output for Test run 7	13
Input and Output for Test run 8	14
Further Information	16
Revision History	16

## Executive Summary

Freqscale.py is a PYTHON program that calculates the optimal scale factors for calculating harmonic vibrational frequencies, fundamental frequencies, and zero-point energies from electronic structure calculations.

## Background Reading and Recommended Citations

1. I. M. Alecu, J. Zheng, Y. Zhao, and D. G. Truhlar, Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries, *Journal of Chemical Theory and Computation* **6**, 2872-2887 (2010). [dx.doi.org/10.1021/ct100326h](https://doi.org/10.1021/ct100326h)
2. H. S. Yu, L. J. Fiedler, I. M. Alecu, and D. G. Truhlar, Computational Thermochemistry: Automated Generation of Scale Factors for Vibrational Frequencies Calculated by Electronic Structure Model Chemistries *Computer Physics Communications*, submitted March 10, 2016.
3. H. S. Yu, L. J. Fiedler, I. M. Alecu, and D. G. Truhlar, Freqscale, version 1 (University of Minnesota, Minneapolis, 2016)

## Usage

There are two models; the “full model” involves optimization of the scale factor against 15 molecules, and the “reduced model” involves optimization against six molecules.

In order to calculate the optimum scale factor for a given method, there are two modes:

1. *Tightly coupled mode*: The user only needs to provide the keyword for a method and basis set in the *Gaussian 09* or *Gaussian 03* program.
2. *Loosely coupled mode*: The user can read in the calculated harmonic zero point energy (ZPE) for six or 15 molecules, as computed previously with any software. Note that the harmonic ZPE is one half the sum of the harmonic frequencies. The ZPE should be in units of kcal/mol, where  $1 \text{ cm}^{-1} = 0.002859144 \text{ kcal/mol}$ , or  $1 \text{ kcal/mol} = 349.7551 \text{ cm}^{-1}$ .

## Package

There are seven files included in the package, which includes five PYTHON programs. The seven files are Freqscale.py, input.py, input6.py, pbs.py, pbs6.py, one bash script called run.sh, and this manual.

## Platform

The program has been tested on the following platform:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

## Installation

The source code is a compressed tar file named `Freqscale.tar.gz`.

To uncompress, enter `gunzip Freqscale.tar.gz`

The uncompressed file will be named `Freqscale.tar`. Extracting the files from the tar file can be done with the command:

```
tar xvf Freqscale.tar
```

As a result, a new directory, `Freqscale`, is created. This directory contains all the files included in the package, as follows:

`Freqscale.py`, `input.py`, `input6`, `pbs.py`, `pbs6`, `run.sh`, and manual of the program

## Examples of running the program

Test runs 1, 2, 7, and 8 do not require using the *Gaussian* program. Test runs 3-6 are for users who do have the *Gaussian* program.

Test run 1 is an example of loosely coupled mode with the full model and a built-in basis set.

The ZPEs are reading from the keyboard.

Test run 2 is an example of loosely coupled mode with the reduced model and a built-in basis set. The ZPEs are reading from the keyboard.

Test run 3 is an example of tightly coupled mode with the full model and a built-in basis set for machines that do not have a PBS job queue system.

Test run 4 is an example of tightly coupled mode with the reduced model and a built-in basis set for machines that do not have a PBS job queue system.

Test run 5 is an example of tightly coupled mode with the full model and a user-defined basis set for machines that have a PBS job queue system.

Test run 6 is an example of tightly coupled mode with the reduced model and a built-in basis set for machines that have a PBS job queue system.

Test run 7 is an example of loosely coupled mode with the full model and a built-in basis set. The ZPEs are reading from a txt file called `freqcom.txt`.

Test run 8 is an example of loosely coupled mode with the reduced model and a built-in basis set. The ZPEs are reading from a txt file called `freqcom.txt`.

**Running the tests:**

- 1) Go to the Freqscale directory you created by running command “tar xvf Freqscale.tar”, and run the bash script by using command “./run.sh”.
- 2) The program will ask you questions, and the user should type the answer to each by using the keyboard. Examples of input and output are given below.

**Test run 1**

Users who do not use *Gaussian* software can run the program directly with pre-calculated harmonic zero-point energies reading from the keyboard. Below we give sample input and output.

***Sample input for Test run 1***

Do you have access to Gaussian software on your machine (yes or no)? > no  
 Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4  
 (This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)  
 reduced model or full model? > full model  
 Reading ZPEs from a pre-created file (yes or no)? > no  
 Please enter the calculated ZPE for the following molecules: c2h2 ch4 co2 co f2 h2co h2o h2 hcn hf n2o n2 nh3 oh cl2

17.04419  
 27.82555  
 7.56411  
 3.19420  
 1.53884  
 16.52225  
 13.52640  
 6.15991  
 10.31873  
 6.00950  
 7.29928  
 3.51917  
 21.43009  
 5.36671  
 0.81906

(Here we choose the ZPE calculated by M06 functional with aug-cc-pVTZ basis set.)

***Sample output for Test run 1***

FREQ: A PROGRAM FOR OPTIMIZING SCALE FACTORS (Version 1)

written by

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Scale Factor for Zero-Point Energies = 0.98304793613100572

Scale Factor for Harmonic Frequencies = 0.99681060723683979

Scale Factor for Fundamental Frequencies = 0.95748868979159951

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. *J. Chem. Theory Comput.* 2010, 6, 2872
2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.*, submitted 2016

**Test run 2**

Users who do not use *Gaussian* software can run the program directly with pre-calculated zero-point energies reading from the keyboard. Below we give sample input and output.

***Sample input for Test run 2***

```

Do you have access to Gaussian software on your machine (yes or no)? > no
Download the python3/3.4 or higher using proper command on your machine > module load
python3/3.4
(This command may differ depending on how the user sets up the environmental variables for using
Python scripts; this may not be necessary if using a standard UNIX system.)
reduced model or full model? > reduced model
Reading ZPEs from a pre-created file (yes or no)? > no
Please enter the calculated ZPE for the following molecules: c2h2 ch4 h2co h2o n2o nh3
17.04419
27.82555
16.52225
13.52640
7.29928
21.43009
(Here we choose the ZPE calculated by M06 functional with aug-cc-pVTZ basis set.)

```

***Sample output for Test run 2***

FREQ: A PROGRAM FOR OPTIMIZING SCALE FACTORS (Version 1)

written by

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Scale Factor for Zero-Point Energies = 0.98424431267694845

Scale Factor for Harmonic Frequencies = 0.99802373305442571

Scale Factor for Fundamental Frequencies = 0.95865396054734775

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. *J. Chem. Theory Comput.* 2010, 6, 2872
2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.*, submitted 2016

### Test run 3

Users who do use *Gaussian* software but do not have a PBS job queue system can run the program directly with pre-calculated zero-point energies in freqcom.txt. Below we give sample input and output.

#### *Sample input for Test run 3*

Do you have access to Gaussian software on your machine (yes or no)? > yes

Download the Gaussian software using proper command on your machine > module load gaussian  
(This command may differ depending on how the user sets up the environmental variables for running *Gaussian* calculations.)

Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4

(This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)

*(If Gaussian software and Python are already installed in the user's machine then hit space to skip the above two questions)*

reduced model or full model? "full model"

Which method are you going to choose? "M06"

Which basis set are you going to choose? "aug-cc-pVTZ"

What is the path of your basis set? Hit the enter key.

Do you have a PBS job queue system (yes or no)? > no

Type in the command for running gaussian calculations on your machine > g09

(This will run Gaussian calculations requiring a short amount of time to complete.)

Running g09 c2h2...

Running g09 ch4...

Running g09 co2...

Running g09 co...

Running g09 f2...

Running g09 h2co...

Running g09 h2o...

Running g09 h2...

Running g09 hcn...

Running g09 hf...

Running g09 n2o...

Running g09 n2...

Running g09 nh3...

Running g09 oh...

Running g09 cl2...

#### *Sample output for Test run 3*

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written by

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Scale Factor for Harmonic Frequencies = 0.99681060723683979

Scale Factor for Fundamental Frequencies = 0.95748868979159951

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. *J. Chem. Theory Comput.* 2010, 6, 2872
2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.*, submitted 2016



## Test run 4

Users who do use Gaussian software but do not have a PBS job queue system can run the program directly with pre-calculated zero-point energies in freqcom.txt. Below we give sample input and output.

### *Sample input for Test run 4*

Do you have access to Gaussian software on your machine (yes or no)? > yes  
 Download the Gaussian software using proper command on your machine > module load gaussian  
 (This command may differ depending on how the user sets up the environmental variables for running Gaussian calculations.)  
 Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4  
 (This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)  
*(If Gaussian software and Python are already installed in the user's machine then hit space to skip the above two questions)*  
 reduced model or full model? "reduced model"  
 Which method are you going to choose? "M06"  
 Which basis set are you going to choose? "aug-cc-pVTZ"  
 What is the path of your basis set? Hit the enter key.  
 Do you have a PBS job queue system (yes or no)? > no  
 Type in the command for running gaussian calculations on your machine > g09  
 (This will run Gaussian calculations requiring a short amount of time to complete.)  
 Running g09 c2h2...  
 Running g09 ch4...  
 Running g09 h2co...  
 Running g09 h2o...  
 Running g09 n2o...  
 Running g09 nh3...

### *Sample output for Test run 4*

FREQ: A PROGRAM FOR OPTIMIZING SCALE FACTORS (Version 1)

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Scale Factor for Zero-Point Energies = 0.9842443126769485

Scale Factor for Harmonic Frequencies = 0.9980237330544257

Scale Factor for Fundamental Frequencies = 0.9586539605473477

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. J. Chem. Theory Comput. 2010, 6, 2872

## Test run 5

- 1) Make sure that the officially distributed *Gaussian 09* or *Gaussian 03* program is properly installed. If you will only use the loosely coupled mode, skip this step.
- 2) Check that *Python* (version 3.4 or higher) is installed.

### *Sample questions and keyboard input for Test run 5*

Do you have access to Gaussian software on your machine (yes or no)? > yes

Download the Gaussian software using proper command on your machine > module load gaussian  
(This command may differ depending on how the user sets up the environmental variables for running *Gaussian* calculations.)

Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4

(This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)

*(If Gaussian software and Python are already installed in the user's machine then hit space to skip the above two questions)*

reduced model or full model? "full model"

Which method are you going to choose? "M06"

Which basis set are you going to choose? "Gen"

What is the path of your basis set? @/home/truhlard/yuhaoyu/research/basis\_set/mg3s.gbs

(This is an example, the path to your external basis set file will differ)

Do you have a PBS job queue system (yes or no)? > yes

(This will submit *Gaussian* calculations to the job queue requiring a short amount of time to complete.)

1468811.mesabim3.msi.umn.edu

1468812.mesabim3.msi.umn.edu

1468813.mesabim3.msi.umn.edu

1468814.mesabim3.msi.umn.edu

1468815.mesabim3.msi.umn.edu

1468816.mesabim3.msi.umn.edu

1468817.mesabim3.msi.umn.edu

1468818.mesabim3.msi.umn.edu

1468819.mesabim3.msi.umn.edu

1468820.mesabim3.msi.umn.edu

1468821.mesabim3.msi.umn.edu

1468822.mesabim3.msi.umn.edu

1468823.mesabim3.msi.umn.edu

1468824.mesabim3.msi.umn.edu

1468825.mesabim3.msi.umn.edu

### *Sample output for Test run 5*

(The following results will be printed to the screen once the calculations are finished. The output should match the following zero-point energies and frequencies as follows.)

## FREQ: A PROGRAM FOR OPTIMIZING SCALE FACTORS (Version 1)

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Scale Factor for Zero-Point Energies = 0.9809435263191598

Scale Factor for Harmonic Frequencies = 0.994676735687628

Scale Factor for Fundamental Frequencies = 0.9554389946348616

## CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. J. Chem. Theory Comput. 2010, 6, 2872
2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. Comput. Phys. Commun. submitted 2016

**Test run 6**

1) Make sure that the officially distributed *Gaussian 09* or *Gaussian 03* program is properly installed. If you will only use the loosely coupled mode, skip this step.

2) Check that *Python* (version 3.4 or higher) is installed.

***Sample input for Test run 6***

Do you have access to Gaussian software on your machine (yes or no)? > yes

Download the Gaussian software using proper command on your machine > module load gaussian  
(This command may differ depending on how the user sets up the environmental variables for running *Gaussian* calculations.)

Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4

(This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)

*(If Gaussian software and Python are already installed in the user's machine then hit space to skip the above two questions)*

Reduced Model or Full Model? "reduced model"

Which method are you going to choose? "M06"

Which basis set are you going to choose? "aug-cc-pVTZ"

What is the path of your basis set? Hit the enter key.

Do you have a PBS job queue system (yes or no)? > yes

1466810.mesabim3.msi.umn.edu

1466811.mesabim3.msi.umn.edu

1466812.mesabim3.msi.umn.edu

1466813.mesabim3.msi.umn.edu

1466814.mesabim3.msi.umn.edu

1466815.mesabim3.msi.umn.edu

***Sample output for Test run 6***

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Scale Factor for Zero-Point Energies = 0.9842443126769485

Scale Factor for Harmonic Frequencies = 0.9980237330544257

Scale Factor for Fundamental Frequencies = 0.9586539605473477

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. *J. Chem. Theory Comput.* 2010, 6, 2872

2. Yu, S.H., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.* submitted 2016

**Test run 7**

Users who do not use *Gaussian* software and who wish to enter frequencies in a file rather than by the keyboard can run the program directly with pre-calculated zero-point energies in a file named freqcom.txt. Below we give sample input and output.

Before running the program please create a text .txt file named “freqcom.txt” with the following ZPEs for these molecules: c2h2 ch4 h2co h2o n2o nh3, e.g. (these test values are for method + basis set *M06/aug-cc-pVTZ*)

freqcom.txt:

17.04419  
27.82555  
16.52225  
13.52640  
7.29928  
21.43009

***Sample input for Test run 7***

Do you have access to Gaussian software on your machine (yes or no)? > no

Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4

(This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)

reduced model or full model? > reduced model

(Here we choose the ZPE calculated by *M06 functional with aug-cc-pVTZ basis set.*)

Reading ZPEs from a pre-created file (yes or no)? > yes

Reading ZPEs from file freqcom.txt

***Sample output for Test run 7***

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Scale Factor for Harmonic Frequencies = 0.99802373305442571

Scale Factor for Fundamental Frequencies = 0.95865396054734775

CITATIONS:

1. Alecu, I.M., Zheng, J., Zhao, Y., and Truhlar, D.G. *J. Chem. Theory Comput.* 2010, 6, 2872
2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.*, submitted 2016

**Test run 8**

Users who do not use *Gaussian* software and who wish to enter frequencies in a file rather than by the keyboard can run the program directly with pre-calculated zero-point energies in a file named freqcom.txt. Below we give sample input and output.

Before running the program please create a text .txt file named “freqcom.txt” with the following ZPEs for these molecules: c2h2 ch4 co2 co f2 h2co h2o h2 hcn hf n2o n2 nh3 oh cl2, e.g. (these test values are for method + basis set *M06/aug-cc-pVTZ*)

freqcom.txt:

17.04419  
 27.82555  
 7.56411  
 3.19420  
 1.53884  
 16.52225  
 13.52640  
 6.15991  
 10.31873  
 6.00950  
 7.29928  
 3.51917  
 21.43009  
 5.36671  
 0.81906

***Sample input for Test run 8***

Do you have access to Gaussian software on your machine (yes or no)? > no

Download the python3/3.4 or higher using proper command on your machine > module load python3/3.4

(This command may differ depending on how the user sets up the environmental variables for using Python scripts; this may not be necessary if using a standard UNIX system.)

reduced model or full model? > full model

(Here we choose the ZPE calculated by M06 functional with aug-cc-pVTZ basis set.)

Reading ZPEs from a pre-created file (yes or no)? > yes

Reading ZPEs from file freqcom.txt

***Sample output for Test run 8***

FREQ: A PROGRAM FOR OPTIMIZING SCALE FACTORS (Version 1)

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Scale Factor for Zero-Point Energies = 0.98304793613100572

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2. Yu, H.S., Fiedler, L.J., Alecu, I.M., and Truhlar, D.G. *Comput. Phys. Commun.*, submitted 2016

**Further information**

To check for updates and news, see [http://comp.chem.umn.edu/freq\\_scale](http://comp.chem.umn.edu/freq_scale)

If assistance is needed, please contact Haoyu Yu at [yuhaoyuapp@gmail.com](mailto:yuhaoyuapp@gmail.com)

**Revision History**

*Version 1*, May 26, 2016

Authors: Haoyu S. Yu, Lucas J. Fiedler, I. M. Alecu, and Donald G. Truhlar