

Converting Between Gaussian Versions

[MGCF](#) - College of Chemistry, University of California, Berkeley

Gaussian chk files contain the raw information associated with a calculation, and we often want to restart new calculations from this information. If you want to start a new calculation based on a chk file from a different Gaussian version, there is an issue: chk files have binary format (which is not human-readable), and in general chk files from different Gaussian versions are not directly compatible. To get around this, we can (1) convert a chk file to fchk format, which is a readable text file, and then (2) convert the fchk file to chk format corresponding to the desired Gaussian version.

For **step (1)**, we need to use the **formchk** utility. Each Gaussian version comes with its own formchk version, so you'll need to choose the one for the Gaussian version that was used to produce the old chk file that you have, or the closest version to it. Here is a list of different formchk versions at MGCF:

```
-----  
/usr/software/gaussian/g03.revD01/formchk          (Gaussian03 32 bit)  
/usr/software/gaussian/g03_64.RevE01/g03/formchk    (Gaussian03 64 bit)  
  
/usr/software/gaussian/g09.revC01/formchk           (Gaussian09 ver C01)  
  
/usr/software/gaussian16/g16.revA03_sse4_2/g16/formchk (Gaussian16 ver A03)  
-----
```

To convert the old chk to fchk format, open a terminal and go to the location of the chk file, and type **/path_to_formchk/formchk filename.chk**, substituting in one of the above full paths to a formchk version, and your actual chk filename. Alternatively, you can first set up the terminal environment for the appropriate Gaussian version, and then simply type **formchk filename.chk**. For example, typing `g03_d01_setup` will set up the environment for G03 rev D01. Note that `g09_setup` is for rev D01, but this formchk version crashes on our systems, so use the above rev C01 version instead.

For **step (2)**, we need to use the **unfchk** utility. For this, choose the unfchk version corresponding to the Gaussian version you want to use in the new calculation. In general, unfchk is found in the same directory as formchk. For example, `/usr/software/gaussian16/g16.revA03_sse4_2/g16/unfchk` may be used to convert a fchk to chk in G16 format. To convert from fchk to chk, type **/path_to_unfchk/unfchk filename.fchk**, where you should use one of the paths listed above for the formchk examples, e.g. `/usr/software/gaussian16/g16.revA03_sse4_2/g16/unfchk`. Again, you can alternatively first set

up the terminal environment for the intended Gaussian version, and then simply type **unfchk filename.fchk**. For example, typing g16_setup will make it so that the unfchk for Gaussian 16 rev A03 is used. Note that formchk and unfchk will not change the prefix for the newly created files, so it's best to rename the newly created fchk file before converting it to the new chk file, otherwise the original chk file will get overwritten by the new chk file.

Here is an example command sequence, for converting an old G09 chk file to a G16 chk file:

```
/usr/software/gaussian/g09.revC01/formchk g09calc.chk  
g16_setup  
cp g09calc.fchk g16calc.fchk  
unfchk g16calc.fchk
```

This produces g16calc.chk, which is compatible with Gaussian 16.

Note also that G09 chk files can be opened in Gaussview6.

There is also the **c8616** utility, which will convert an older-version chk file to a G16 chk file. It is run by typing **c8616 filename.chk**, and is accessible after typing g16_setup, or by applying the same path as used above for G16's formchk and unfchk. And there is also the **c8609** utility, which converts older-version chk files to G09 format (either use g09_setup or type in the full path as used above for G09 formchk). These utilities don't change the file prefix, so they'll overwrite the original chk file.