

# Gaussian

## Category: Licensed Application Software

Gaussian 03 is a suite of electronic structure programs. It is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.

For more information, please see the [Gaussian manual](#) or the [Gaussian web site](#).

Two versions (c.02 and e.01) of Gaussian 03 have been installed on Columbia systems. To use the older c.02 version, do the following in your PBS script:

```
module load gaussian.03.c02
source $g03root/g03/bsd/g03.login
```

```
g03 input output
```

To use the newer e.01 version (built with **intel-comp.10.0.023** and **intel-mkl.9.1.023**), do:

```
module load gaussian.03.e.01
source $g03root/g03/bsd/g03.login
```

```
g03 input output
```

If you are a bash user, then do:

```
. /usr/share/modules/init/bash
module load gaussian.03.e.01
. $g03root/g03/bsd/g03.profile
```

```
g03 input output
```

See also: <http://en.wikipedia.org/wiki/GAUSSIAN>

Article ID: 123

Last updated: 17 Jul, 2012

Computing at NAS -> Software Environment -> Licensed Application Software -> Gaussian  
<http://www.nas.nasa.gov/hecc/support/kb/entry/123/?ajax=1>