FCC (Facio Cartesian Coordinate) Format
for
Computational Chemistry

A new chemical file format, FCC (Facio Cartesian Coordinate) has been created in order to store Cartesian coordinates of GAMESS or Gaussian calculation without any truncation of the values and complete connectivity of the compound.

The following example of FCC is created based on a $H2O$ calculated with Gaussian.

```
Facio Cartesian Coordinate :  C:¥G03W¥Facio¥H2O.out
3
   O      1      0.0000000000      0.1146870000      0.0000000000      2      3
   H      2      0.7540650000     -0.4587490000      0.0000000000      1
   H      3     -0.7540650000     -0.4587490000      0.0000000000      1
```

The 1st line should contain string "Facio Cartesian Coordinate". You can write a comment after the colon of the 1st line. The 2nd line contains the number of atoms. After the 3rd line, each contains a kind of the atom, serial number, Cartesian coordinates and connectivity in the following format.

A3, I7, 3(F17.10), n(I7)   (where n is the number of bonds and varies from 0 to 8)

Cartesian coordinates can be saved as a number which has 10 digits after the decimal point. This feature is useful for recording Cartesian coordinates of GAMESS or Gaussian outputs. The connectivity data is also useful for complete reconstruction of the structure. Thus, FCC (Facio Cartesian Coordinate) is suitable chemical file format of computational chemistry.