STEP BY STEP TUTORIAL. MASS SPECTRUM OF CH3F MOLECULE
Operative system: CentOS
Queue system: SLURM

```
-----------------------------------------------------------------
DEPENDENCIES

  1) jmol (version >= 12.2 )
     This is already installed on QUBuntu
  2) gnuplot (version >= 4.2)
     This is already installed on QUBuntu
  3) gawk (version >= 3.1)
     This is not installed on QUBuntu
       $ sudo apt-get install gawk
  4) gwenview or other image viewer for displaying a collection
     of images
     This is not installed on QUBuntu
       $ sudo apt-get install gwenview
  5) Download the following files from moodle:
        M3C-1.0-intelc-14.0.3-i686.tar.gz
        gamess-i686.tar.gz
        CCC-utils.tar.gz
-----------------------------------------------------------------

user@hostname:~$ cd $HOME
user@hostname:~$ ls
CCC-utils.tar.gz   gamess-x86_64.tar.gz   M3C-1.0-intelc-14.0.3-x86_64.tar.gz

-----------------------------------------------------------------
Installing GAMESS
-----------------------------------------------------------------

user@hostname:~$ tar xfz  gamess-x86_64.tar.gz
user@hostname:~$ ls
CCC-utils.tar.gz   gamess  gamess-x86_64.tar.gz   M3C-1.0-intelc-14.0.3-x86_64.tar.gz
user@hostname:~$ mv gamess .gamess

-----------------------------------------------------------------
Installing M3C
-----------------------------------------------------------------

user@hostname:~$ tar xfz M3C-1.0-intelc-14.0.3-i686.tar.gz
user@hostname:~$ ls
CCC-utils.tar.gz   gamess-x86_64.tar.gz  M3C  M3C-1.0-intelc-14.0.3-x86_64.tar.gz
user@hostname:~$ mv M3C .M3C
user@hostname:~$ vim .bash_profile

<APPEND THE NEXT TWO LINES>

export M3C_HOME=$HOME/.M3C/
export PATH=$M3C_HOME/bin:$PATH

-----------------------------------------------------------------
Installing CCC-utils
-----------------------------------------------------------------

user@hostname:~$ tar xfz CCC-utils.tar.gz
user@hostname:~$ ls
CCC.properties   CCC.utils.sh   CCC-utils.tar.gz   gamess-x86_64.tar.gz  M3C  M3C-1.0-intelc-14.0.3-x86_64.tar.gz
user@hostname:~$ mv CCC.properties .CCC.properties
user@hostname:~$ mv CCC.utils.sh .CCC.utils.sh
user@hostname:~$ vim .bash_profile

<APPEND THE NEXT LINE>

source ~/.CCC.utils.sh

-----------------------------------------------------------------
Work space Setup.
-----------------------------------------------------------------

<OPEN A NEW TERMINAL WINDOW>

user@hostname:~$ cp -r .M3C/examples/ M3C-examples
user@hostname:~$ ls
gamess-i686.tar.gz  M3C-1.0-intelc-14.0.3-i686.tar.gz  M3C-examples
```

```
user@hostname:~$ cd M3C-examples/

user@hostname:~/M3C-examples$ ls
b3lyp.optg-GAMESS.inp  diMethylFluoride  b3lyp.freqs-GAMESS.inp  methylFluoride  pm3.optg-GAMESS.inp  reactorT.m3c

-----------------------------------------------------------------
The tutorial itself.
-----------------------------------------------------------------

user@hostname:~/M3C-examples$ cd methylFluoride/
user@hostname:~/M3C-examples/methylFluoride$ ls
CH3F+.m3c  fragments.inp  init

user@hostname$ M3C.fragments H3,C,F
H, C, F, H2, HC, HF, CF, H3, H2C, H2F, HCF, H3C, H3F, H2CF, H3CF

user@hostname:~/M3C-examples/methylFluoride$ cd init
user@hostname:~/M3C-examples/methylFluoride/init$ M3C.viewXYZ
CF.xyz ... OK
C.xyz ... OK
F.xyz ... OK
H2CF.xyz ... OK
H2C.xyz ... OK
H2F.xyz ... OK
H2.xyz ... OK
H3CF.xyz ... OK
H3C.xyz ... OK
H3F.xyz ... OK
H3.xyz ... OK
HCF.xyz ... OK
HC.xyz ... OK
HF.xyz ... OK
H.xyz ... OK

user@hostname:~/M3C-examples/methylFluoride/init$ ls
CF.gif  C.gif  F.gif  H2CF.gif  H2C.gif  H2F.gif  H2.gif  H3CF.gif  H3C.gif  H3F.gif  H3.gif  HCF.gif  HC.gif  HF.gif  H.gif
CF.xyz  C.xyz  F.xyz  H2CF.xyz  H2C.xyz  H2F.xyz  H2.xyz  H3CF.xyz  H3C.xyz  H3F.xyz  H3.xyz  HCF.xyz  HC.xyz  HF.xyz  H.xyz
user@hostname:~/M3C-examples/methylFluoride/init$ gwenview . &
user@hostname:~/M3C-examples/methylFluoride/init$ cd ..

user@hostname:~/M3C-examples/methylFluoride$ CCC.M3C-gamess.geniso fragments.inp ../pm3.optg-GAMESS.inp ../reactorT.m3c 5 init results
Submitted batch job 885757

user@hostname:~/M3C-examples/methylFluoride$ squeue -u $USER
  JOBID  PARTITION      USER    STATE       TIME     NODELIST CPU                                                                  NAME
 885757       bigp  naguirre  RUNNING       4:19      fosforo   4                                  ~/M3C-WorkSpace/examples/methylFluoride/

<AFTER 5 MINUTES>

user@hostname:~/M3C-examples/methylFluoride$ cat CCC.log
Running:          F,         C,        CF,         H ... OK     Time elapsed: 0h 0m 33s
Running:         HF,        HC,       HCF,        H2 ... OK     Time elapsed: 0h 0m 28s
Running:        H2F,       H2C,      H2CF,        H3 ... OK     Time elapsed: 0h 0m 34s
Running:        H3F,       H3C,         F,         C ... OK     Time elapsed: 0h 0m 44s
Running:         CF,         H,        HF,        HC ... OK     Time elapsed: 0h 0m 26s
Running:        HCF,        H2,       H2F,       H2C ... OK     Time elapsed: 0h 0m 32s
Running:       H2CF,        H3,       H3F,       H3C ... OK     Time elapsed: 0h 0m 35s
Running:       H3CF                                  ... OK     Time elapsed: 0h 0m 41s
                                                                        Total: 0h 4m 33s

user@hostname:~/M3C-examples/methylFluoride$ ls
CCC.err  CCC.log  CH3F+.m3c  fragments.inp  init  log  results

user@hostname:~/M3C-examples/methylFluoride$ cd results/
user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.xyz     H2CF.q1.m1-1.xyz  H2F.q1.m1-1.xyz   H3C.q0.m2-3.xyz  H3.q0.m2-2.xyz   HC.q0.m2-1.xyz    history-C.q1.m2     history-H2F.q0.m2  history-H3F.q0.m1  history-HC.q1.m1
CF.q1.m1-1.xyz     H2CF.q1.m1-2.xyz  H2.q0.m1-1.xyz    H3C.q1.m1-1.xyz  H3.q0.m2-3.xyz  HC.q1.m1-1.xyz    history-F.q0.m2     history-H2F.q1.m1  history-H3F.q1.m2  history-HF.q0.m1
C.q0.m1-1.xyz      H2CF.q1.m1-3.xyz  H2.q1.m2-1.xyz     H3C.q1.m1-2.xyz  H3.q0.m2-4.xyz  HF.q0.m1-1.xyz    history-F.q1.m1     history-H2.q0.m1   history-H3.q0.m2   history-HF.q1.m2
C.q1.m2-1.xyz      H2C.q0.m1-1.xyz   H3CF.q1.m2-1.xyz  H3F.q0.m1-1.xyz  H3.q1.m1-1.xyz   HF.q1.m2-1.xyz    history-H2CF.q0.m2  history-H2.q1.m2   history-H3.q1.m1   history-H.q0.m2
F.q0.m2-1.xyz      H2C.q1.m2-1.xyz   H3CF.q1.m2-2.xyz  H3F.q1.m2-1.xyz  HCF.q0.m1-1.xyz  history-CF.q0.m2  history-H2CF.q1.m1  history-H3CF.q1.m2  history-HCF.q0.m1  history-H.q1.m0
F.q1.m1-1.xyz      H2F.q0.m2-1.xyz   H3C.q0.m2-1.xyz    H3F.q1.m2-2.xyz  HCF.q1.m2-1.xyz  history-CF.q1.m1  history-H2C.q0.m1   history-H3C.q0.m2  history-HCF.q1.m2  H.q0.m2-1.xyz
H2CF.q0.m2-1.xyz   H2F.q0.m2-3.xyz   H3C.q0.m2-2.xyz   H3.q0.m2-1.xyz   HCF.q1.m2-2.xyz  history-C.q0.m1   history-H2C.q1.m2   history-H3C.q1.m1  history-HC.q0.m2   H.q1.m0-1.xyz

user@hostname:~/M3C-examples/methylFluoride/results$ rm -rf history-*
user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.xyz  F.q0.m2-1.xyz     H2CF.q1.m1-2.xyz  H2F.q0.m2-1.xyz  H2.q1.m2-1.xyz    H3C.q0.m2-2.xyz  H3F.q0.m1-1.xyz  H3.q0.m2-2.xyz  HCF.q0.m1-1.xyz  HC.q1.m1-1.xyz  H.q1.m0-1.xyz
CF.q1.m1-1.xyz  F.q1.m1-1.xyz     H2CF.q1.m1-3.xyz  H2F.q0.m2-3.xyz  H3CF.q1.m2-1.xyz  H3C.q0.m2-3.xyz  H3F.q1.m2-1.xyz  H3.q0.m2-3.xyz  HCF.q1.m2-1.xyz  HF.q0.m1-1.xyz
C.q0.m1-1.xyz   H2CF.q0.m2-1.xyz  H2C.q0.m1-1.xyz   H2F.q1.m1-1.xyz  H3CF.q1.m2-2.xyz  H3C.q1.m1-1.xyz  H3F.q1.m2-2.xyz  H3.q0.m2-4.xyz  HCF.q1.m2-2.xyz  HF.q1.m2-1.xyz
C.q1.m2-1.xyz   H2CF.q1.m1-1.xyz  H2C.q1.m2-1.xyz   H2.q0.m1-1.xyz   H3C.q0.m2-1.xyz   H3C.q1.m1-2.xyz  H3.q0.m2-1.xyz   H3.q1.m1-1.xyz  HC.q0.m2-1.xyz   H.q0.m2-1.xyz

user@hostname:~/M3C-examples/methylFluoride/results$ M3C.viewXYZ
CF.q0.m2-1.xyz ... OK
```

```
CF.q1.m1-1.xyz ... OK
C.q0.m1-1.xyz ... OK
C.q1.m2-1.xyz ... OK
F.q0.m2-1.xyz ... OK
F.q1.m1-1.xyz ... OK
H2CF.q0.m2-1.xyz ... OK
H2CF.q1.m1-1.xyz ... OK
H2CF.q1.m1-2.xyz ... OK
H2CF.q1.m1-3.xyz ... OK
H2C.q0.m1-1.xyz ... OK
H2C.q1.m2-1.xyz ... OK
H2F.q0.m2-1.xyz ... OK
H2F.q0.m2-3.xyz ... OK
H2F.q1.m1-1.xyz ... OK
H2.q0.m1-1.xyz ... OK
H2.q1.m2-1.xyz ... OK
H3CF.q1.m2-1.xyz ... OK
H3CF.q1.m2-2.xyz ... OK
H3C.q0.m2-1.xyz ... OK
H3C.q0.m2-2.xyz ... OK
H3C.q0.m2-3.xyz ... OK
H3C.q1.m1-1.xyz ... OK
H3C.q1.m1-2.xyz ... OK
H3F.q0.m1-1.xyz ... OK
H3F.q1.m2-1.xyz ... OK
H3F.q1.m2-2.xyz ... OK
H3.q0.m2-1.xyz ... OK
H3.q0.m2-2.xyz ... OK
H3.q0.m2-3.xyz ... OK
H3.q0.m2-4.xyz ... OK
H3.q1.m1-1.xyz ... OK
HCF.q0.m1-1.xyz ... OK
HCF.q1.m2-1.xyz ... OK
HCF.q1.m2-2.xyz ... OK
HC.q0.m2-1.xyz ... OK
HC.q1.m1-1.xyz ... OK
HF.q0.m1-1.xyz ... OK
HF.q1.m2-1.xyz ... OK
H.q0.m2-1.xyz ... OK
H.q1.m0-1.xyz ... OK

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.gif  F.q0.m2-1.gif     H2CF.q1.m1-2.gif  H2F.q0.m2-1.gif  H2.q1.m2-1.gif    H3C.q0.m2-2.gif  H3F.q0.m1-1.gif  H3.q0.m2-2.gif  HCF.q0.m1-1.gif  HC.q1.m1-1.gif  H.q1.m0-1.gif
CF.q0.m2-1.xyz  F.q0.m2-1.xyz     H2CF.q1.m1-2.xyz  H2F.q0.m2-1.xyz  H2.q1.m2-1.xyz    H3C.q0.m2-2.xyz  H3F.q0.m1-1.xyz  H3.q0.m2-2.xyz  HCF.q0.m1-1.xyz  HC.q1.m1-1.xyz  H.q1.m0-1.xyz
CF.q1.m1-1.gif  F.q1.m1-1.gif     H2CF.q1.m1-3.gif  H2F.q0.m2-3.gif  H3CF.q1.m2-1.gif  H3C.q0.m2-3.gif  H3F.q1.m2-1.gif  H3.q0.m2-3.gif  HCF.q1.m2-1.gif  HF.q0.m1-1.gif
CF.q1.m1-1.xyz  F.q1.m1-1.xyz     H2CF.q1.m1-3.xyz  H2F.q0.m2-3.xyz  H3CF.q1.m2-1.xyz  H3C.q0.m2-3.xyz  H3F.q1.m2-1.xyz  H3.q0.m2-3.xyz  HCF.q1.m2-1.xyz  HF.q0.m1-1.xyz
C.q0.m1-1.gif   H2CF.q0.m2-1.gif  H2C.q0.m1-1.gif   H2F.q1.m1-1.gif  H3CF.q1.m2-2.gif  H3C.q1.m1-1.gif  H3F.q1.m2-2.gif  H3.q0.m2-4.gif  HCF.q1.m2-2.gif  HF.q1.m2-1.gif
C.q0.m1-1.xyz   H2CF.q0.m2-1.xyz  H2C.q0.m1-1.xyz   H2F.q1.m1-1.xyz  H3CF.q1.m2-2.xyz  H3C.q1.m1-1.xyz  H3F.q1.m2-2.xyz  H3.q0.m2-4.xyz  HCF.q1.m2-2.xyz  HF.q1.m2-1.xyz
C.q1.m2-1.gif   H2CF.q1.m1-1.gif  H2C.q1.m2-1.gif   H2.q0.m1-1.gif   H3C.q0.m2-1.gif   H3C.q1.m1-2.gif  H3.q0.m2-1.gif   H3.q1.m1-1.gif  HC.q0.m2-1.gif   H.q0.m2-1.gif
C.q1.m2-1.xyz   H2CF.q1.m1-1.xyz  H2C.q1.m2-1.xyz   H2.q0.m1-1.xyz   H3C.q0.m2-1.xyz   H3C.q1.m1-2.xyz  H3.q0.m2-1.xyz   H3.q1.m1-1.xyz  HC.q0.m2-1.xyz   H.q0.m2-1.xyz

user@hostname:~/M3C-examples/methylFluoride/results$ gwenview . &
```

<REMOVE MOLECULES WHICH ARE SEPARATED IN TWO OR MORE PIECES>

```
user@hostname:~/M3C-examples/methylFluoride/results$ rm H2CF.q1.m1-2.* H2F.q0.m2-1.* H2F.q0.m2-3.* H3.q0.m2-* H3C.q0.m2-2.* H3C.q0.m2-3.* H3C.q1.m1-2.*
user@hostname:~/M3C-examples/methylFluoride/results$ rm H3CF.q1.m2-2.* H3F.q0.m1-1.* H3F.q1.m2-1.* H3F.q1.m2-2.*
user@hostname:~/M3C-examples/methylFluoride/results$ rm *.gif

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.xyz  C.q1.m2-1.xyz  H2CF.q0.m2-1.xyz  H2C.q0.m1-1.xyz  H2.q0.m1-1.xyz    H3C.q0.m2-1.xyz  HCF.q0.m1-1.xyz  HC.q0.m2-1.xyz  HF.q1.m2-1.xyz
CF.q1.m1-1.xyz  F.q0.m2-1.xyz  H2CF.q1.m1-1.xyz  H2C.q1.m2-1.xyz  H2.q1.m2-1.xyz    H3C.q1.m1-1.xyz  HCF.q1.m2-1.xyz  HC.q1.m1-1.xyz  H.q0.m2-1.xyz
C.q0.m1-1.xyz   F.q1.m1-1.xyz  H2CF.q1.m1-3.xyz  H2F.q1.m1-1.xyz  H3CF.q1.m2-1.xyz  H3.q1.m1-1.xyz   HCF.q1.m2-2.xyz  HF.q0.m1-1.xyz  H.q1.m0-1.xyz

user@hostname:~/M3C-examples/methylFluoride/results$ cp -r ../results ../results.backup

user@hostname:~/M3C-examples/methylFluoride/results$ CCC.M3C-gamess.optg bigp ../../b3lyp.optg-GAMESS.inp
Submitted batch job  885760

user@hostname:~/M3C-examples/methylFluoride$ squeue -u $USER
  JOBID  PARTITION      USER    STATE       TIME     NODELIST CPU                                                                 NAME
 885760       bigp  naguirre  RUNNING       0:16      fosforo   4                                ~/M3C-WorkSpace/examples/methylFluoride/results/
```

<AFTER 17 MINUTES>

```
user@hostname:~/M3C-examples/methylFluoride$ cat CCC.log
Running:      CF.q0.m2-1,     CF.q1.m1-1,      C.q0.m1-1,      C.q1.m2-1 ... OK     Time elapsed: 0h 0m 34s
Running:       F.q0.m2-1,      F.q1.m1-1,   H2CF.q0.m2-1,   H2CF.q1.m1-1 ... OK     Time elapsed: 0h 1m 24s
Running:    H2CF.q1.m1-3,    H2C.q0.m1-1,    H2C.q1.m2-1,    H2F.q1.m1-1 ... OK     Time elapsed: 0h 7m 23s
Running:      H2.q0.m1-1,     H2.q1.m2-1,   H3CF.q1.m2-1,    H3C.q0.m2-1 ... OK     Time elapsed: 0h 5m 12s
Running:     H3C.q1.m1-1,     H3.q1.m1-1,    HCF.q0.m1-1,    HCF.q1.m2-1 ... OK     Time elapsed: 0h 1m 22s
Running:     HCF.q1.m2-2,     HC.q0.m2-1,     HC.q1.m1-1,     HF.q0.m1-1 ... OK     Time elapsed: 0h 0m 46s
Running:      HF.q1.m2-1,      H.q0.m2-1,      H.q1.m0-1                   ... OK     Time elapsed: 0h 0m 10s
```

```
                                                                                                              Total: 0h 16m 51s

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CCC.err          C.q0.m1-1.xyz    F.q1.m1-1.xyz      H2CF.q1.m1-3.xyz   H2F.q1.m1-1.xyz    H3CF.q1.m2-1.xyz   H3.q1.m1-1.xyz    HCF.q1.m2-2.xyz   HF.q0.m1-1.xyz    H.q1.m0-1.xyz
CCC.log          C.q0.m1-1.xyz0   F.q1.m1-1.xyz0     H2CF.q1.m1-3.xyz0  H2F.q1.m1-1.xyz0   H3CF.q1.m2-1.xyz0  H3.q1.m1-1.xyz0   HCF.q1.m2-2.xyz0  HF.q0.m1-1.xyz0   H.q1.m0-1.xyz0
CF.q0.m2-1.xyz   C.q1.m2-1.xyz    H2CF.q0.m2-1.xyz   H2C.q0.m1-1.xyz    H2.q0.m1-1.xyz     H3C.q0.m2-1.xyz    HCF.q0.m1-1.xyz   HC.q0.m2-1.xyz    HF.q1.m2-1.xyz    log
CF.q0.m2-1.xyz0  C.q1.m2-1.xyz0   H2CF.q0.m2-1.xyz0  H2C.q0.m1-1.xyz0   H2.q0.m1-1.xyz0    H3C.q0.m2-1.xyz0   HCF.q0.m1-1.xyz0  HC.q0.m2-1.xyz0   HF.q1.m2-1.xyz0
CF.q1.m1-1.xyz   F.q0.m2-1.xyz    H2CF.q1.m1-1.xyz   H2C.q1.m2-1.xyz    H2.q1.m2-1.xyz     H3C.q1.m1-1.xyz    HCF.q1.m2-1.xyz   HC.q1.m1-1.xyz    H.q0.m2-1.xyz
CF.q1.m1-1.xyz0  F.q0.m2-1.xyz0   H2CF.q1.m1-1.xyz0  H2C.q1.m2-1.xyz0   H2.q1.m2-1.xyz0    H3C.q1.m1-1.xyz0   HCF.q1.m2-1.xyz0  HC.q1.m1-1.xyz0   H.q0.m2-1.xyz0

user@hostname:~/M3C-examples/methylFluoride/results$ M3C.viewXYZ
CF.q0.m2-1.xyz ... OK
CF.q1.m1-1.xyz ... OK
C.q0.m1-1.xyz ... OK
C.q1.m2-1.xyz ... OK
F.q0.m2-1.xyz ... OK
F.q1.m1-1.xyz ... OK
H2CF.q0.m2-1.xyz ... OK
H2CF.q1.m1-1.xyz ... OK
H2CF.q1.m1-3.xyz ... OK
H2C.q0.m1-1.xyz ... OK
H2C.q1.m2-1.xyz ... OK
H2F.q1.m1-1.xyz ... OK
H2.q0.m1-1.xyz ... OK
H2.q1.m2-1.xyz ... OK
H3CF.q1.m2-1.xyz ... OK
H3C.q0.m2-1.xyz ... OK
H3C.q1.m1-1.xyz ... OK
H3.q1.m1-1.xyz ... OK
HCF.q0.m1-1.xyz ... OK
HCF.q1.m2-1.xyz ... OK
HCF.q1.m2-2.xyz ... OK
HC.q0.m2-1.xyz ... OK
HC.q1.m1-1.xyz ... OK
HF.q0.m1-1.xyz ... OK
HF.q1.m2-1.xyz ... OK
H.q0.m2-1.xyz ... OK
H.q1.m0-1.xyz ... OK

user@hostname:~/M3C-examples/methylFluoride/results$ gwenview . &
```

<REMOVE MOLECULES WHICH ARE SEPARATED IN TWO OR MORE PIECES>

```
user@hostname:~/M3C-examples/methylFluoride/results$ ls
CCC.err          C.q0.m1-1.xyz    F.q1.m1-1.xyz      H2CF.q1.m1-3.xyz   H2F.q1.m1-1.xyz0   H3CF.q1.m2-1.xyz0  H3.q1.m1-1.xyz0   HCF.q1.m2-2.xyz0  HF.q0.m1-1.xyz0   H.q1.m0-1.xyz0
CCC.log          C.q0.m1-1.xyz0   F.q1.m1-1.xyz0     H2CF.q1.m1-3.xyz0  H2.q0.m1-1.gif     H3C.q0.m2-1.gif    HCF.q0.m1-1.gif   HC.q0.m2-1.gif    HF.q1.m2-1.gif    log
CF.q0.m2-1.gif   C.q1.m2-1.gif    H2CF.q0.m2-1.gif   H2C.q0.m1-1.gif    H2.q0.m1-1.xyz     H3C.q0.m2-1.xyz    HCF.q0.m1-1.xyz   HC.q0.m2-1.xyz    HF.q1.m2-1.xyz
CF.q0.m2-1.xyz   C.q1.m2-1.xyz    H2CF.q0.m2-1.xyz   H2C.q0.m1-1.xyz    H2.q0.m1-1.xyz0    H3C.q0.m2-1.xyz0   HCF.q0.m1-1.xyz0  HC.q0.m2-1.xyz0   HF.q1.m2-1.xyz0
CF.q0.m2-1.xyz0  C.q1.m2-1.xyz0   H2CF.q0.m2-1.xyz0  H2C.q0.m1-1.xyz0   H2.q1.m2-1.gif     H3C.q1.m1-1.gif    HCF.q1.m2-1.gif   HC.q1.m1-1.gif    H.q0.m2-1.gif
CF.q1.m1-1.gif   F.q0.m2-1.gif    H2CF.q1.m1-1.gif   H2C.q1.m2-1.gif    H2.q1.m2-1.xyz     H3C.q1.m1-1.xyz    HCF.q1.m2-1.xyz   HC.q1.m1-1.xyz    H.q0.m2-1.xyz
CF.q1.m1-1.xyz   F.q0.m2-1.xyz    H2CF.q1.m1-1.xyz   H2C.q1.m2-1.xyz    H2.q1.m2-1.xyz0    H3C.q1.m1-1.xyz0   HCF.q1.m2-1.xyz0  HC.q1.m1-1.xyz0   H.q0.m2-1.xyz0
CF.q1.m1-1.xyz0  F.q0.m2-1.xyz0   H2CF.q1.m1-1.xyz0  H2C.q1.m2-1.xyz0   H3CF.q1.m2-1.gif   H3.q1.m1-1.gif     HCF.q1.m2-2.gif   HF.q0.m1-1.gif    H.q1.m0-1.gif
C.q0.m1-1.gif    F.q1.m1-1.gif    H2CF.q1.m1-3.gif   H2F.q1.m1-1.xyz    H3CF.q1.m2-1.xyz   H3.q1.m1-1.xyz     HCF.q1.m2-2.xyz   HF.q0.m1-1.xyz    H.q1.m0-1.xyz

user@hostname:~/M3C-examples/methylFluoride/results$ cp -r ../results ../results.backup2

user@hostname:~/M3C-examples/methylFluoride/results$ CCC.M3C-gamess.freqs bigp ../../b3lyp.freqs-GAMESS.inp
Submitted batch job 885764

user@hostname:~/M3C-examples/methylFluoride$ squeue -u $USER
  JOBID  PARTITION      USER    STATE       TIME     NODELIST CPU                                                      NAME
 885764       bigp  naguirre  RUNNING       0:12      fosforo   4                                 ~/M3C-WorkSpace/examples/methylFluoride/results/
```

<AFTER 14 MINUTES>

```
user@hostname:~/M3C-examples/methylFluoride$ cat CCC.log
Running:      CF.q0.m2-1,      CF.q1.m1-1,       C.q0.m1-1,      C.q1.m2-1 ... OK     Time elapsed: 0h 0m 47s
Running:       F.q0.m2-1,       F.q1.m1-1,    H2CF.q0.m2-1,   H2CF.q1.m1-1 ... OK     Time elapsed: 0h 2m 49s
Running:    H2CF.q1.m1-3,     H2C.q0.m1-1,     H2C.q1.m2-1,    H2F.q1.m1-1 ... OK     Time elapsed: 0h 2m 3s
Running:      H2.q0.m1-1,      H2.q1.m2-1,    H3CF.q1.m2-1,    H3C.q0.m2-1 ... OK     Time elapsed: 0h 4m 30s
Running:     H3C.q1.m1-1,      H3.q1.m1-1,     HCF.q0.m1-1,    HCF.q1.m2-1 ... OK     Time elapsed: 0h 1m 44s
Running:     HCF.q1.m2-2,      HC.q0.m2-1,      HC.q1.m1-1,     HF.q0.m1-1 ... OK     Time elapsed: 0h 1m 34s
Running:      HF.q1.m2-1,       H.q0.m2-1,       H.q1.m0-1                 ... OK     Time elapsed: 0h 0m 21s
                                                                                                Total: 0h 13m 48s

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CCC.err          C.q0.m1-1.rxyz  F.q1.m1-1.gif      H2CF.q1.m1-1.xyz0  H2C.q1.m2-1.xyz   H2.q1.m2-1.xyz     H3C.q1.m1-1.rxyz  HCF.q1.m2-1.gif   HC.q0.m2-1.xyz0   HF.q1.m2-1.xyz
CCC.log          C.q0.m1-1.xyz   F.q1.m1-1.rxyz     H2CF.q1.m1-3.gif   H2C.q1.m2-1.xyz0  H2.q1.m2-1.xyz0    H3C.q1.m1-1.xyz   HCF.q1.m2-1.rxyz  HC.q1.m1-1.gif    HF.q1.m2-1.xyz0
CF.q0.m2-1.gif   C.q0.m1-1.xyz0  F.q1.m1-1.xyz      H2CF.q1.m1-3.rxyz  H2F.q1.m1-1.rxyz  H3CF.q1.m2-1.gif   H3C.q1.m1-1.xyz0  HCF.q1.m2-1.xyz   HC.q1.m1-1.rxyz   H.q0.m2-1.gif
CF.q0.m2-1.rxyz  C.q1.m2-1.gif   F.q1.m1-1.xyz0     H2CF.q1.m1-3.xyz   H2F.q1.m1-1.xyz   H3CF.q1.m2-1.rxyz  H3.q1.m1-1.gif    HCF.q1.m2-1.xyz0  HC.q1.m1-1.xyz    H.q0.m2-1.rxyz
CF.q0.m2-1.xyz   C.q1.m2-1.rxyz  H2CF.q0.m2-1.gif   H2CF.q1.m1-3.xyz0  H2F.q1.m1-1.xyz0  H3CF.q1.m2-1.xyz   H3.q1.m1-1.rxyz   HCF.q1.m2-2.gif   HC.q1.m1-1.xyz0   H.q0.m2-1.xyz
CF.q0.m2-1.xyz0  C.q1.m2-1.xyz   H2CF.q0.m2-1.rxyz  H2C.q0.m1-1.gif    H2.q0.m1-1.gif    H3CF.q1.m2-1.xyz0  H3.q1.m1-1.xyz    HCF.q1.m2-2.rxyz  HF.q0.m1-1.gif    H.q0.m2-1.xyz0
```

```
CF.q1.m1-1.gif   C.q1.m2-1.xyz0  H2CF.q0.m2-1.xyz   H2C.q0.m1-1.rxyz   H2.q0.m1-1.rxyz   H3C.q0.m2-1.gif    H3.q1.m1-1.xyz0   HCF.q1.m2-2.xyz   HF.q0.m1-1.rxyz  H.q1.m0-1.gif
CF.q1.m1-1.rxyz  F.q0.m2-1.gif   H2CF.q0.m2-1.xyz0  H2C.q0.m1-1.xyz    H2.q0.m1-1.xyz    H3C.q0.m2-1.rxyz   HCF.q0.m1-1.gif   HCF.q1.m2-2.xyz0  HF.q0.m1-1.xyz   H.q1.m0-1.rxyz
CF.q1.m1-1.xyz   F.q0.m2-1.rxyz  H2CF.q1.m1-1.gif   H2C.q0.m1-1.xyz0   H2.q0.m1-1.xyz0   H3C.q0.m2-1.xyz    HCF.q0.m1-1.rxyz  HC.q0.m2-1.gif    HF.q0.m1-1.xyz0  H.q1.m0-1.xyz
CF.q1.m1-1.xyz0  F.q0.m2-1.xyz   H2CF.q1.m1-1.rxyz  H2C.q1.m2-1.gif    H2.q1.m2-1.gif    H3C.q0.m2-1.xyz0   HCF.q0.m1-1.xyz   HC.q0.m2-1.rxyz   HF.q1.m2-1.gif   H.q1.m0-1.xyz0
C.q0.m1-1.gif    F.q0.m2-1.xyz0  H2CF.q1.m1-1.xyz   H2C.q1.m2-1.rxyz   H2.q1.m2-1.rxyz   H3C.q1.m1-1.gif    HCF.q0.m1-1.xyz0  HC.q0.m2-1.xyz    HF.q1.m2-1.rxyz  log
```

user@hostname:~/M3C-examples/methylFluoride/results$ cat H3CF.q1.m2-1.rxyz

```
5
Energy = -139.2533771353
C    0.1154628047    0.1877491323   -0.1667164707
F    0.3783270368   -0.0400309891    1.3734139624
H    1.2567980800    0.1336840239    1.7112768867
H    0.1133346434    1.2632628110   -0.3095801253
H   -0.6162625649   -0.5781749781   -0.3952342532

FREQUENCIES    9
3532.89
3346.10
3125.53
1330.99
1067.59
906.93
834.50
566.22
166.30
```

user@hostname:~/M3C-examples/methylFluoride/results$ grep -H "^I" *.rxyz

<THERE ARE NOT MOLECULE WITH IMAGINARY FREQUENCIES, OTHERWISE YOU WOULD HAVE TO DELETE THEIR ASSOCIATED FILES (.xyz, .xyz0, .rxyz, .gif)>

user@hostname:~/M3C-examples/methylFluoride/results$ cp -r ../results ../results.backup3
user@hostname:~/M3C-examples/methylFluoride/results$ cp ../CH3F+.m3c .

user@hostname:~/M3C-examples/methylFluoride/results$ M3C.makeDB CH3F+.m3c

```
BEGIN FRAGMENTS_DATABASE
        #-------------------------------------------------------------------------------------------------
        #          Label    Z  M  L  SYM              geomFile              Eelec               maxVib
        #-------------------------------------------------------------------------------------------------
                  H(d1)    0  2  0    1         H.q0.m2-1.rxyz          -13.572100
                  C(s1)    0  1  0    1         C.q0.m1-1.rxyz        -1027.790000
                  F(d1)    0  2  0    1         F.q0.m2-1.rxyz        -2713.690000
                 H2(s1)    0  1  0    1        H2.q0.m1-1.rxyz          -31.833900         H(d1)+H(d1)
                 HC(d1)    0  2  0    1        HC.q0.m2-1.rxyz        -1046.730000         H(d1)+C(s1)
                 HF(s1)    0  1  0    1        HF.q0.m1-1.rxyz        -2732.950000         H(d1)+F(d1)
                 CF(d1)    0  2  0    1        CF.q0.m2-1.rxyz        -3748.880000         C(s1)+F(d1)
                H2C(s1)    0  1  0    1       H2C.q0.m1-1.rxyz        -1064.370000        H(d1)+HC(d1)
                HCF(s1)    0  1  0    1       HCF.q0.m1-1.rxyz        -3765.840000        H(d1)+CF(d1)
                H3C(d1)    0  2  0    1       H3C.q0.m2-1.rxyz        -1083.470000       H2(s1)+HC(d1)
               H2CF(d1)    0  2  0    1      H2CF.q0.m2-1.rxyz        -3783.830000       H2(s1)+CF(d1)
                  Hp(1)    1  0  0    1         H.q1.m0-1.rxyz            0.000000
                  Cp(d1)   1  2  0    1         C.q1.m2-1.rxyz        -1018.080000
                  Fp(s1)   1  1  0    1         F.q1.m1-1.rxyz        -2692.420000
                 H2p(d1)   1  2  0    1        H2.q1.m2-1.rxyz          -16.298600         Hp(1)+H(d1)
                 HCp(s1)   1  1  0    1        HC.q1.m1-1.rxyz        -1035.860000        H(d1)+Cp(d1)
                 HFp(d1)   1  2  0    1        HF.q1.m2-1.rxyz        -2716.870000         Hp(1)+F(d1)
                 CFp(s1)   1  1  0    1        CF.q1.m1-1.rxyz        -3739.460000        Cp(d1)+F(d1)
                 H3p(s1)   1  1  0    1        H3.q1.m1-1.rxyz          -35.977800        Hp(1)+H2(s1)
                H2Cp(d1)   1  2  0    1       H2C.q1.m2-1.rxyz        -1054.540000       H2(s1)+Cp(d1)
                HCFp(d1)   1  2  0    1       HCF.q1.m2-1.rxyz        -3753.040000       Cp(d1)+HF(s1)
                HCFp(d2)   1  2  0    1       HCF.q1.m2-2.rxyz        -3755.850000       H(d1)+CFp(s1)
                H3Cp(s1)   1  1  0    1       H3C.q1.m1-1.rxyz        -1073.720000      H(d1)+H2Cp(d1)
               H2CFp(s1)   1  1  0    1      H2CF.q1.m1-1.rxyz        -3774.770000       HCp(s1)+HF(s1)
               H2CFp(s3)   1  1  0    1      H2CF.q1.m1-3.rxyz        -3770.520000       H(d1)+HCFp(d2)
               H3CFp(d1)   1  2  0    1      H3CF.q1.m2-1.rxyz        -3789.280000      H(d1)+H2CFp(s1)
        #-------------------------------------------------------------------------------------------------
END FRAGMENTS_DATABASE
```

<THE NEXT STEP IS TO REPLACE THE PREVIOUSLY GENERATED BLOCK BY THE EQUIVALENT ONE IN THE CH3F+.m3c FILE>
<THE M3C FILE IS READY TO BE EXECUTED>

user@hostname:~/M3C-examples/methylFluoride/results$ M3C -i CH3F+.m3c

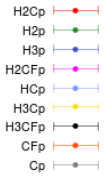
```
 Input file = CH3F+.m3c

Blocks input file
-----------------
> BEGIN GOPTIONS
>     systemRadius = 8.0
>     overlappingRadius = 0.4
>     useRandomWalkers = FALSE

...
```

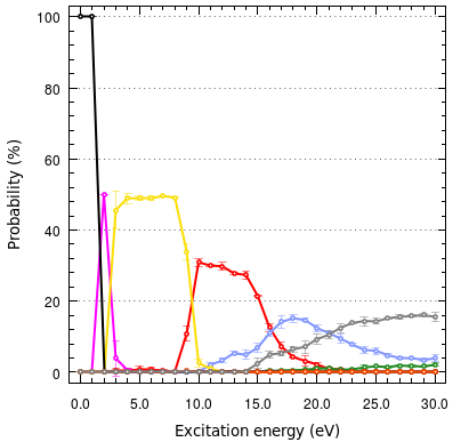
```
 ---------------------------------------------------------------------------
 START TIME: Thu Feb  5 23:59:22 2015
 ---------------------------------------------------------------------------

                      GOptions:zero =        0.10E-11
                GOptions:systemRadius =         8.00000 A
        GOptions:randomWalkStepRadius =         1.00000 A
                  GOptions:printLevel =     1
                  GOptions:debugLevel =     1


     +-----------------------------------+
     | FRAGMENTS DATABASE INITIALIZATION |
     +-----------------------------------+


              file name = H.q0.m2-1.rxyz
                   name = H(d1)
     Moments of inertia = [       0.00000       0.00000       0.00000  ]   amu*angs**2
     Moments of inertia = [       0.00000       0.00000       0.00000  ]   a.u.
                 Radius =         0.37000   A
                  Eelec =     -13.5721000   eV
                  Eelec =      -0.4987653   a.u.
                   Mass =       1.0080000   amu
              (fr, fv) = (    0    0  )
                 maxEvib =       0.0000000   eV

...

     +---------------------------------------+
     | END FRAGMENTS DATABASE INITIALIZATION |
     +---------------------------------------+


                        reactives = H3CFp(d1)
                 excitationEnergy =        10.00000 eV
                   numberOfEvents =           10000
              numberOfExperiments =               2
                             task = V,T,S:0,V,T,S:1:-1
        geometryHistoryFilePrefix = geom
                freqBlockingCheck =               4
                            track = energy

#-------------------------------------
# ENERGY HISTORY
#-------------------------------------
#             trans       intermol           elec            vib            rot            tot     formula
#                eV             eV             eV             eV             eV             eV
#           -------       -------       --------       -------        -------        -------
 aV         4.03427       0.00000    -3787.41000       3.01840        1.07732    -3779.28000     H3Cp(s1)+F(d1)
 pT         1.70911       0.00000    -3787.41000       5.34357        1.07732    -3779.28000     H3Cp(s1)+F(d1)
 rS         2.11221       0.00000    -3787.41000       4.94047        1.07732    -3779.28000     H3Cp(s1)+F(d1)
 rV         1.57511       0.00000    -3787.41000       4.87930        1.67559    -3779.28000     H3Cp(s1)+F(d1)

...

#-------------------------------------
# Channels histogram
#-------------------------------------
#             item         1         2           aver      desv
#                       -----     -----          ----      ----
          H3Cp+F       0.121     0.095          0.108     0.013
          H+H2Cp+F     0.606     0.549          0.578     0.029
          H2+HCp+F     0.273     0.356          0.315     0.042


#                         item         1         2           aver      desv
#                                     -----     -----          ----      ----
          H2(s1)+HCp(s1)+F(d1)     0.273     0.356          0.315     0.042
          H(d1)+H2Cp(d1)+F(d1)     0.606     0.549          0.578     0.029
          H3Cp(s1)+F(d1)           0.121     0.095          0.108     0.013

...

 ---------------------------------------------------------------------------
 ELAPSED TIME:            0 h           0 m          12 s
 END TIME: Thu Feb  5 23:59:34 2015
 ---------------------------------------------------------------------------
```

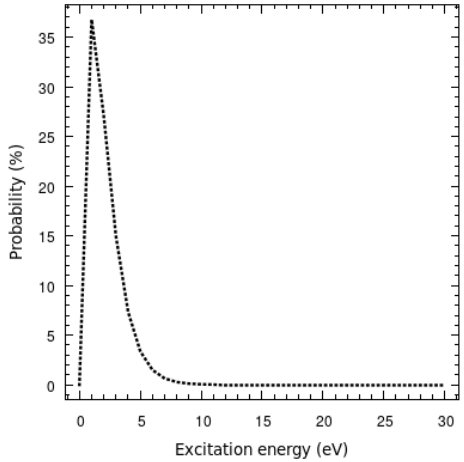
user@hostname$ M3C.analysis CH3F+.m3c energy
user@hostname$ M3C.analysis CH3F+.m3c ecorr Et.vs.Ev
user@hostname$ M3C.analysis CH3F+.m3c ecorr Er.vs.Ev
user@hostname$ M3C.analysis CH3F+.m3c ecorr Er.vs.Et

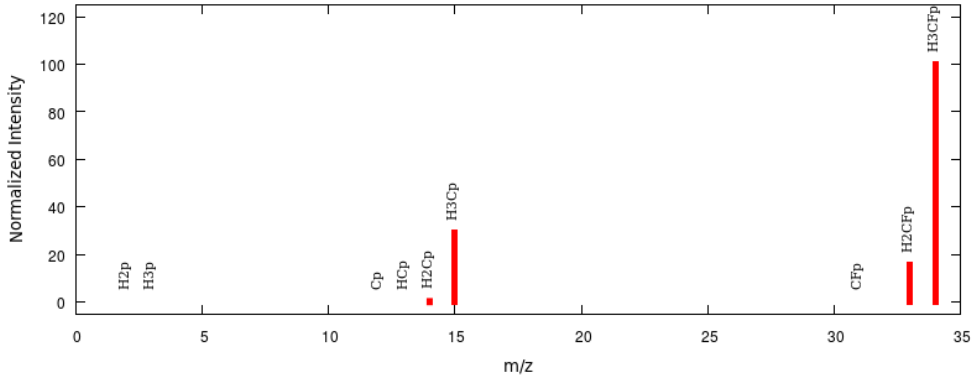
```
user@hostname$ M3C.analysis CH3F+.m3c species
user@hostname$ M3C.analysis CH3F+.m3c channels

<CHANGE “tracking = energy” BY “tracking = none” IN CH3F+.m3c FILE IN ORDER TO SAVE EXECUTION TIME>

user@hostname:~/results$ M3C.p normalp -i CH3F+.m3c
Submitted batch job 886456

user@hostname:~/M3C-examples/methylFluoride$ squeue -u $USER
  JOBID  PARTITION      USER    STATE       TIME     NODELIST CPU                                                                                NAME
 886456    normalp  naguirre  RUNNING       0:44      silicio   4                                ~/M3C-WorkSpace/examples/methylFluoride/results/

<AFTER 5 MINUTES>

user@hostname:~/M3C-examples/methylFluoride$ cat CCC.log
Running:    0.00000,   1.00000,   2.00000,   3.00000 ... OK     Time elapsed: 0h 0m 18s
Running:    4.00000,   5.00000,   6.00000,   7.00000 ... OK     Time elapsed: 0h 0m 15s
Running:    8.00000,   9.00000,  10.00000,  11.00000 ... OK     Time elapsed: 0h 0m 21s
Running:   12.00000,  13.00000,  14.00000,  15.00000 ... OK     Time elapsed: 0h 0m 24s
Running:   16.00000,  17.00000,  18.00000,  19.00000 ... OK     Time elapsed: 0h 0m 30s
Running:   20.00000,  21.00000,  22.00000,  23.00000 ... OK     Time elapsed: 0h 0m 34s
Running:   24.00000,  25.00000,  26.00000,  27.00000 ... OK     Time elapsed: 0h 0m 34s
Running:   28.00000,  29.00000,  30.00000             ... OK     Time elapsed: 0h 0m 34s
                                                                        Total: 0h 3m 31s

user@hostname:~/M3C-examples/methylFluoride/results$ M3C.analysis CH3F+.m3c fit_sBR

...

 ### ERROR ### M3CfitBR: HCFp has not been mapped.
                        Remove it from the input file

...

<THIS ERROR MEANS THAT HCF+ MOLECULE IS NOT INTO THE CALCULATED SET OF FRAGMENTS>
<IN ORDER TO FIX IT, COMMENT OUT THE LINE “HCFp     4.4     0.0   32.0” AND/OR MORE LINES AS REQUIRED BY USING THE CHARACTER #>

user@hostname:~/M3C-examples/methylFluoride/results$ M3C.analysis CH3F+.m3c fit_sBR
user@hostname:~/M3C-examples/methylFluoride/results$ M3C.analysis CH3F+.m3c fit_sfE
user@hostname:~/M3C-examples/methylFluoride/results$ M3C.analysis CH3F+.m3c S.vs.E “p”
```

RESULT


H2Cp
H2p
H3p
H2CFp
HCp
H3Cp
H3CFp
CFp
Cp


Probability (%)
Excitation energy (eV)
0
20
40
60
80
100
0.0
5.0
10.0
15.0
20.0
25.0
30.0


Probability (%)
Excitation energy (eV)
0
5
10
15
20
25
30
35


Normalized Intensity
m/z
H2p
H3p
Cp
HCp
H2Cp
H3Cp
CFp
H2CFp
H3CFp
0
20
40
60
80
100
120
0
5
10
15
20
25
30
35