STEP BY STEP TUTORIAL. MASS SPECTRUM OF CH3F MOLECULE
Operating system: QUBuntu

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-----------------------------------------------------------------------
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
-----------------------------------------------------------------------
```

```
user@hostname:~$ cd $HOME
user@hostname:~$ ls
gamess.tar.gz   M3C-1.0-intelc-14.0.3-i686.tar.gz
```

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-----------------------------------------------------------------------
Installing GAMESS
-----------------------------------------------------------------------
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```
user@hostname:~$ tar xfz  gamess-i686.tar.gz
user@hostname:~$ ls
gamess  gamess-i686.tar.gz  M3C-1.0-intelc-14.0.3-i686.tar.gz
user@hostname:~$ mv gamess .gamess
user@hostname:~$ vim .bashrc

<APPEND THE NEXT LINE>

export PATH=$HOME/.gamess:$PATH
```

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-----------------------------------------------------------------------
Installing M3C
-----------------------------------------------------------------------
```

```
user@hostname:~$ tar xfz M3C-1.0-intelc-14.0.3-i686.tar.gz
user@hostname:~$ ls
gamess-i686.tar.gz  M3C  M3C-1.0-intelc-14.0.3-i686.tar.gz
user@hostname:~$ mv M3C .M3C
user@hostname:~$ vim .bashrc

<APPEND THE NEXT TWO LINES>

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

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-----------------------------------------------------------------------
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
```

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-----------------------------------------------------------------------
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$ M3C-gamess.geniso fragments.inp ../pm3.optg-GAMESS.inp ../reactorT.m3c 5 init results
Running:          F,          C ... OK     Time elapsed: 0h 0m 0s
Running:         CF,          H ... OK     Time elapsed: 0h 0m 23s
Running:         HF,         HC ... OK     Time elapsed: 0h 0m 37s
Running:        HCF,         H2 ... OK     Time elapsed: 0h 0m 48s
Running:        H2F,        H2C ... OK     Time elapsed: 0h 2m 33s
Running:       H2CF,         H3 ... OK     Time elapsed: 0h 1m 6s
Running:        H3F,        H3C ... OK     Time elapsed: 0h 7m 55s
Running:          F,          C ... OK     Time elapsed: 0h 0m 1s
Running:         CF,          H ... OK     Time elapsed: 0h 0m 45s
Running:         HF,         HC ... OK     Time elapsed: 0h 1m 47s
Running:        HCF,         H2 ... OK     Time elapsed: 0h 1m 9s
Running:        H2F,        H2C ... OK     Time elapsed: 0h 2m 17s
Running:       H2CF,         H3 ... OK     Time elapsed: 0h 3m 1s
Running:        H3F,        H3C ... OK     Time elapsed: 0h 3m 43s
Running:       H3CF             ... OK     Time elapsed: 0h 1m 37s
                                                    Total: 0h 27m 42s

user@hostname:~/M3C-examples/methylFluoride$ ls
CH3F+.m3c  fragments.inp  init  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.q1.m1-1.xyz  H3.q0.m2-2.xyz   HC.q1.m1-1.xyz    history-F.q0.m2     history-H2F.q1.m1   history-H3F.q1.m2  history-HF.q0.m1
CF.q1.m1-1.xyz    H2CF.q1.m1-2.xyz  H2.q0.m1-1.xyz    H3C.q1.m1-4.xyz  H3.q0.m2-3.xyz   HF.q0.m1-1.xyz    history-F.q1.m1     history-H2.q0.m1    history-H3.q0.m2   history-HF.q1.m2
C.q0.m1-1.xyz     H2CF.q1.m1-3.xyz  H2.q1.m2-1.xyz    H3C.q1.m1-5.xyz  H3.q0.m2-5.xyz   HF.q1.m2-1.xyz    history-H2CF.q0.m2  history-H2.q1.m2    history-H3.q1.m1   history-H.q0.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   history-CF.q0.m2  history-H2CF.q1.m1  history-H3CF.q1.m2  history-HCF.q0.m1  history-H.q1.m0
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.q1.m1  history-H2C.q0.m1   history-H3C.q0.m2   history-HCF.q1.m2  H.q0.m2-1.xyz
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-C.q0.m1   history-H2C.q1.m2   history-H3C.q1.m1   history-HC.q0.m2   H.q1.m0-1.xyz
H2CF.q0.m2-1.xyz  H2F.q0.m2-2.xyz   H3C.q0.m2-3.xyz   H3.q0.m2-1.xyz   HC.q0.m2-1.xyz   history-C.q1.m2   history-H2F.q0.m2   history-H3F.q0.m1   history-HC.q1.m1

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.m2-3.xyz  H3F.q0.m1-1.xyz  H3.q0.m2-2.xyz  HCF.q0.m1-1.xyz  HF.q0.m1-1.xyz
CF.q1.m1-1.xyz  F.q1.m1-1.xyz     H2CF.q1.m1-3.xyz  H2F.q0.m2-2.xyz  H3CF.q1.m2-1.xyz  H3C.q1.m1-1.xyz  H3F.q1.m2-1.xyz  H3.q0.m2-3.xyz  HCF.q1.m2-1.xyz  HF.q1.m2-1.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.m1-4.xyz  H3F.q1.m2-2.xyz  H3.q0.m2-5.xyz  HC.q0.m2-1.xyz   H.q0.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.m1-5.xyz  H3.q0.m2-1.xyz   H3.q1.m1-1.xyz  HC.q1.m1-1.xyz   H.q1.m0-1.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.m2-2.xyz ... OK
H2F.q1.m1-1.xyz ... OK
H2.q0.m1-1.xyz ... OK
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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.m2-3.xyz ... OK
H3C.q1.m1-1.xyz ... OK
H3C.q1.m1-4.xyz ... OK
H3C.q1.m1-5.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.m2-5.xyz ... OK
H3.q1.m1-1.xyz ... OK
HCF.q0.m1-1.xyz ... OK
HCF.q1.m2-1.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.m2-3.gif  H3F.q0.m1-1.gif  H3.q0.m2-2.gif  HCF.q0.m1-1.gif  HF.q0.m1-1.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.m2-3.xyz  H3F.q0.m1-1.xyz  H3.q0.m2-2.xyz  HCF.q0.m1-1.xyz  HF.q0.m1-1.xyz
CF.q1.m1-1.gif  F.q1.m1-1.gif     H2CF.q1.m1-3.gif  H2F.q0.m2-2.gif  H3CF.q1.m2-1.gif  H3C.q1.m1-1.gif  H3F.q1.m2-1.gif  H3.q0.m2-3.gif  HCF.q1.m2-1.gif  HF.q1.m2-1.gif
CF.q1.m1-1.xyz  F.q1.m1-1.xyz     H2CF.q1.m1-3.xyz  H2F.q0.m2-2.xyz  H3CF.q1.m2-1.xyz  H3C.q1.m1-1.xyz  H3F.q1.m2-1.xyz  H3.q0.m2-3.xyz  HCF.q1.m2-1.xyz  HF.q1.m2-1.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.m1-4.gif  H3F.q1.m2-2.gif  H3.q0.m2-5.gif  HC.q0.m2-1.gif   H.q0.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.m1-4.xyz  H3F.q1.m2-2.xyz  H3.q0.m2-5.xyz  HC.q0.m2-1.xyz   H.q0.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.m1-5.gif  H3.q0.m2-1.gif   H3.q1.m1-1.gif  HC.q1.m1-1.gif   H.q1.m0-1.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.m1-5.xyz  H3.q0.m2-1.xyz   H3.q1.m1-1.xyz  HC.q1.m1-1.xyz   H.q1.m0-1.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.* H2CF.q1.m1-3.* H2F.q0.m2-1.* H2F.q0.m2-2.* H3.q0.m2-2.*
user@hostname:~/M3C-examples/methylFluoride/results$ rm H3.q0.m2-3.* H3C.q0.m2-3.* H3C.q1.m1-4.* H3C.q1.m1-5.* H3F.q*
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.q1.m2-1.xyz  H2.q1.m2-1.xyz    H3C.q0.m2-1.xyz  H3.q0.m2-5.xyz   HCF.q1.m2-1.xyz  HF.q0.m1-1.xyz  H.q1.m0-1.xyz
CF.q1.m1-1.xyz  F.q0.m2-1.xyz  H2CF.q1.m1-1.xyz  H2F.q1.m1-1.xyz  H3CF.q1.m2-1.xyz  H3C.q1.m1-1.xyz  H3.q1.m1-1.xyz   HC.q0.m2-1.xyz   HF.q1.m2-1.xyz
C.q0.m1-1.xyz   F.q1.m1-1.xyz  H2C.q0.m1-1.xyz   H2.q0.m1-1.xyz   H3CF.q1.m2-2.xyz  H3.q0.m2-1.xyz   HCF.q0.m1-1.xyz  HC.q1.m1-1.xyz   H.q0.m2-1.xyz

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

user@hostname:~/M3C-examples/methylFluoride/results$ M3C-gamess.optg ../../b3lyp.optg-GAMESS.inp
Running:      CF.q0.m2-1,     CF.q1.m1-1 ... OK     Time elapsed: 0h 1m 7s
Running:       C.q0.m1-1,      C.q1.m2-1 ... OK     Time elapsed: 0h 0m 0s
Running:       F.q0.m2-1,      F.q1.m1-1 ... OK     Time elapsed: 0h 0m 0s
Running:    H2CF.q0.m2-1,   H2CF.q1.m1-1 ... OK     Time elapsed: 0h 3m 36s
Running:     H2C.q0.m1-1,    H2C.q1.m2-1 ... OK     Time elapsed: 0h 0m 47s
Running:     H2F.q1.m1-1,     H2.q0.m1-1 ... OK     Time elapsed: 0h 0m 19s
Running:      H2.q1.m2-1,   H3CF.q1.m2-1 ... OK     Time elapsed: 0h 8m 31s
Running:    H3CF.q1.m2-2,    H3C.q0.m2-1 ... OK     Time elapsed: 0h 3m 59s
Running:     H3C.q1.m1-1,     H3.q0.m2-1 ... OK     Time elapsed: 0h 1m 51s
Running:      H3.q0.m2-5,     H3.q1.m1-1 ... OK     Time elapsed: 0h 0m 23s
Running:     HCF.q0.m1-1,    HCF.q1.m2-1 ... OK     Time elapsed: 0h 2m 2s
Running:      HC.q0.m2-1,     HC.q1.m1-1 ... OK     Time elapsed: 0h 0m 29s
Running:      HF.q0.m1-1,     HF.q1.m2-1 ... OK     Time elapsed: 0h 0m 19s
Running:       H.q0.m2-1,      H.q1.m0-1 ... OK     Time elapsed: 0h 0m 0s
Running:                                 ... OK     Time elapsed: 0h 0m 0s
                                                                  Total: 0h 23m 23s

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.xyz   C.q1.m2-1.xyz   H2CF.q0.m2-1.xyz   H2C.q1.m2-1.xyz   H2.q1.m2-1.xyz     H3C.q0.m2-1.xyz   H3.q0.m2-5.xyz    HCF.q1.m2-1.xyz   HF.q0.m1-1.xyz   H.q1.m0-1.xyz
CF.q0.m2-1.xyz0  C.q1.m2-1.xyz0  H2CF.q0.m2-1.xyz0  H2C.q1.m2-1.xyz0  H2.q1.m2-1.xyz0     H3C.q0.m2-1.xyz0  H3.q0.m2-5.xyz0    HCF.q1.m2-1.xyz0  HF.q0.m1-1.xyz0  H.q1.m0-1.xyz0
CF.q1.m1-1.xyz   F.q0.m2-1.xyz   H2CF.q1.m1-1.xyz   H2F.q1.m1-1.xyz   H3CF.q1.m2-1.xyz   H3C.q1.m1-1.xyz   H3.q1.m1-1.xyz     HC.q0.m2-1.xyz    HF.q1.m2-1.xyz
CF.q1.m1-1.xyz0  F.q0.m2-1.xyz0  H2CF.q1.m1-1.xyz0  H2F.q1.m1-1.xyz0  H3CF.q1.m2-1.xyz0  H3C.q1.m1-1.xyz0  H3.q1.m1-1.xyz0   HC.q0.m2-1.xyz0   HF.q1.m2-1.xyz0
C.q0.m1-1.xyz    F.q1.m1-1.xyz    H2C.q0.m1-1.xyz    H2.q0.m1-1.xyz    H3CF.q1.m2-2.xyz   H3.q0.m2-1.xyz    HCF.q0.m1-1.xyz   HC.q1.m1-1.xyz    H.q0.m2-1.xyz
C.q0.m1-1.xyz0   F.q1.m1-1.xyz0   H2C.q0.m1-1.xyz0   H2.q0.m1-1.xyz0   H3CF.q1.m2-2.xyz0  H3.q0.m2-1.xyz0   HCF.q0.m1-1.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
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H2CF.q0.m2-1.xyz ... OK
H2CF.q1.m1-1.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
H3CF.q1.m2-2.xyz ... OK
H3C.q0.m2-1.xyz ... OK
H3C.q1.m1-1.xyz ... OK
H3.q0.m2-1.xyz ... OK
H3.q0.m2-5.xyz ... OK
H3.q1.m1-1.xyz ... OK
HCF.q0.m1-1.xyz ... OK
HCF.q1.m2-1.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$ rm H3.q0.m2-1.*

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.gif   C.q0.m1-1.xyz0  F.q1.m1-1.xyz      H2C.q0.m1-1.gif   H2F.q1.m1-1.xyz0  H3CF.q1.m2-1.xyz   H3C.q1.m1-1.gif   HCF.q0.m1-1.gif   HC.q0.m2-1.xyz0  HF.q1.m2-1.xyz
CF.q0.m2-1.xyz   C.q1.m2-1.gif   F.q1.m1-1.xyz0     H2C.q0.m1-1.xyz   H2.q0.m1-1.gif     H3CF.q1.m2-1.xyz0  H3C.q1.m1-1.xyz   HCF.q0.m1-1.xyz   HC.q1.m1-1.gif   HF.q1.m2-1.xyz0
CF.q0.m2-1.xyz0  C.q1.m2-1.xyz   H2CF.q0.m2-1.gif  H2C.q0.m1-1.xyz0  H2.q0.m1-1.xyz     H3CF.q1.m2-2.gif   H3C.q1.m1-1.xyz0  HCF.q0.m1-1.xyz0  HC.q1.m1-1.xyz   H.q0.m2-1.gif
CF.q1.m1-1.gif   C.q1.m2-1.xyz0  H2CF.q0.m2-1.xyz   H2C.q1.m2-1.gif   H2.q0.m1-1.xyz0   H3CF.q1.m2-2.xyz   H3.q0.m2-5.xyz    HCF.q1.m2-1.gif   HC.q1.m1-1.xyz0  H.q0.m2-1.xyz
CF.q1.m1-1.xyz   F.q0.m2-1.gif   H2CF.q0.m2-1.xyz0  H2C.q1.m2-1.xyz   H2.q1.m2-1.gif     H3CF.q1.m2-2.xyz0  H3.q0.m2-5.xyz0   HCF.q1.m2-1.xyz   HF.q0.m1-1.gif   H.q0.m2-1.xyz0
CF.q1.m1-1.xyz0  F.q0.m2-1.xyz   H2CF.q1.m1-1.gif   H2C.q1.m2-1.xyz0  H2.q1.m2-1.xyz     H3C.q0.m2-1.gif    H3.q1.m1-1.gif    HCF.q1.m2-1.xyz0  HF.q0.m1-1.xyz   H.q1.m0-1.gif
C.q0.m1-1.gif    F.q0.m2-1.xyz0  H2CF.q1.m1-1.xyz   H2F.q1.m1-1.gif   H2.q1.m2-1.xyz0   H3C.q0.m2-1.xyz    H3.q1.m1-1.xyz    HC.q0.m2-1.gif    HF.q0.m1-1.xyz0  H.q1.m0-1.xyz
C.q0.m1-1.xyz    F.q1.m1-1.gif   H2CF.q1.m1-1.xyz0  H2F.q1.m1-1.xyz   H3CF.q1.m2-1.gif   H3C.q0.m2-1.xyz0   H3.q1.m1-1.xyz0   HC.q0.m2-1.xyz     HF.q1.m2-1.gif   H.q1.m0-1.xyz0

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

user@hostname:~/M3C-examples/methylFluoride/results$ M3C-gamess.freqs ../../b3lyp.freqs-GAMESS.inp
Running:      CF.q0.m2-1,     CF.q1.m1-1 ... OK     Time elapsed: 0h 2m 1s
Running:       C.q0.m1-1,      C.q1.m2-1 ... OK     Time elapsed: 0h 0m 13s
Running:       F.q0.m2-1,      F.q1.m1-1 ... OK     Time elapsed: 0h 0m 14s
Running:    H2CF.q0.m2-1,   H2CF.q1.m1-1 ... OK     Time elapsed: 0h 8m 3s
Running:     H2C.q0.m1-1,    H2C.q1.m2-1 ... OK     Time elapsed: 0h 2m 23s
Running:     H2F.q1.m1-1,     H2.q0.m1-1 ... OK     Time elapsed: 0h 1m 19s
Running:      H2.q1.m2-1,   H3CF.q1.m2-1 ... OK     Time elapsed: 0h 9m 4s
Running:    H3CF.q1.m2-2,    H3C.q0.m2-1 ... OK     Time elapsed: 0h 11m 11s
Running:     H3C.q1.m1-1,     H3.q0.m2-5 ... OK     Time elapsed: 0h 2m 11s
Running:      H3.q1.m1-1,    HCF.q0.m1-1 ... OK     Time elapsed: 0h 2m 24s
Running:     HCF.q1.m2-1,     HC.q0.m2-1 ... OK     Time elapsed: 0h 3m 31s
Running:      HC.q1.m1-1,     HF.q0.m1-1 ... OK     Time elapsed: 0h 0m 52s
Running:      HF.q1.m2-1,      H.q0.m2-1 ... OK     Time elapsed: 0h 0m 49s
Running:       H.q1.m0-1                ... OK     Time elapsed: 0h 0m 3s
                                                                 Total: 0h 44m 18s

user@hostname:~/M3C-examples/methylFluoride/results$ ls
CF.q0.m2-1.gif   C.q0.m1-1.xyz0  F.q1.m1-1.xyz      H2C.q0.m1-1.rxyz  H2.q0.m1-1.gif     H3CF.q1.m2-1.xyz0  H3C.q1.m1-1.xyz   HCF.q0.m1-1.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     H2C.q0.m1-1.xyz   H2.q0.m1-1.rxyz     H3CF.q1.m2-2.gif   H3C.q1.m1-1.xyz0  HCF.q0.m1-1.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   H2C.q0.m1-1.xyz0  H2.q0.m1-1.xyz     H3CF.q1.m2-2.rxyz  H3.q0.m2-5.rxyz   HCF.q1.m2-1.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.q1.m2-1.gif   H2.q0.m1-1.xyz0   H3CF.q1.m2-2.xyz   H3.q0.m2-5.xyz    HCF.q1.m2-1.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.q1.m2-1.rxyz  H2.q1.m2-1.gif     H3CF.q1.m2-2.xyz0  H3.q0.m2-5.xyz0   HCF.q1.m2-1.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.q1.m2-1.xyz   H2.q1.m2-1.rxyz    H3C.q0.m2-1.gif    H3.q1.m1-1.gif    HCF.q1.m2-1.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.q1.m2-1.xyz0  H2.q1.m2-1.xyz     H3C.q0.m2-1.rxyz   H3.q1.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  H2F.q1.m1-1.gif   H2.q1.m2-1.xyz0   H3C.q0.m2-1.xyz    H3.q1.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   H2F.q1.m1-1.rxyz  H3CF.q1.m2-1.gif   H3C.q0.m2-1.xyz0   H3.q1.m1-1.xyz0   HC.q0.m2-1.xyz     HF.q1.m2-1.rxyz
C.q0.m1-1.rxyz   F.q1.m1-1.gif   H2CF.q1.m1-1.xyz0  H2F.q1.m1-1.xyz   H3CF.q1.m2-1.rxyz   H3C.q1.m1-1.gif    HCF.q0.m1-1.gif   HC.q0.m2-1.xyz0   HF.q1.m2-1.xyz
C.q0.m1-1.xyz    F.q1.m1-1.rxyz  H2C.q0.m1-1.gif    H2F.q1.m1-1.xyz0  H3CF.q1.m2-1.xyz   H3C.q1.m1-1.rxyz   HCF.q0.m1-1.rxyz   HC.q1.m1-1.gif    HF.q1.m2-1.xyz0

user@hostname:~/M3C-examples/methylFluoride/results$ cat H3CF.q1.m2-2.rxyz
5
Energy = -139.2622142579
C   0.5063172279   -0.2100414032   -0.1685057135
F   -0.2546710826   0.7995943914   0.0969352537
H   0.1557351925   -1.1353725153   0.4524849110
H   0.7554782499   -0.3594035325   -1.2172639004
H   1.3649855324   -0.2706254204   0.6195076992

FREQUENCIES    9
3202.02
2555.74
```

```
2212.72
1461.16
1285.72
1092.85
1056.26
966.02
733.31

user@hostname:~/M3C-examples/methylFluoride/results$ grep -H "^I" *.rxyz
H2F.q1.m1-1.rxyz:I
H2F.q1.m1-1.rxyz:I

<THIS MOLECULE HAS TWO IMAGINARY FREQUENCIES, THEN YOU HAVE TO DELETE THEIR RELATED FILES>

user@hostname:~/M3C-examples/methylFluoride/results$ rm H2F.q1.m1-1.*
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)
               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       H2(s1)+CFp(s1)
              H3CFp(d1)     1  2  0    1      H3CF.q1.m2-1.rxyz       -3789.280000      H(d1)+H2CFp(s1)
              H3CFp(d2)     1  2  0    1      H3CF.q1.m2-2.rxyz       -3789.520000      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: Wed Jan 14 16:10:45 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          16 s
 END TIME: Wed Jan 14 16:11:01 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 -i CH3F+.m3c
Running:    0.00000,   1.00000 ... OK     Time elapsed: 0h 0m 12s
Running:    2.00000,   3.00000 ... OK     Time elapsed: 0h 0m 22s
Running:    4.00000,   5.00000 ... OK     Time elapsed: 0h 0m 21s
Running:    6.00000,   7.00000 ... OK     Time elapsed: 0h 0m 23s
Running:    8.00000,   9.00000 ... OK     Time elapsed: 0h 0m 25s
Running:   10.00000,  11.00000 ... OK     Time elapsed: 0h 0m 40s
Running:   12.00000,  13.00000 ... OK     Time elapsed: 0h 0m 35s
Running:   14.00000,  15.00000 ... OK     Time elapsed: 0h 0m 40s
Running:   16.00000,  17.00000 ... OK     Time elapsed: 0h 0m 45s
Running:   18.00000,  19.00000 ... OK     Time elapsed: 0h 0m 50s
```

```
Running:    20.00000,  21.00000 ... OK     Time elapsed: 0h 0m 50s
Running:    22.00000,  23.00000 ... OK     Time elapsed: 0h 0m 57s
Running:    24.00000,  25.00000 ... OK     Time elapsed: 0h 0m 57s
Running:    26.00000,  27.00000 ... OK     Time elapsed: 0h 0m 54s
Running:    28.00000,  29.00000 ... OK     Time elapsed: 0h 0m 57s
Running:    30.00000            ... OK     Time elapsed: 0h 0m 32s
                                                 Total: 0h 10m 20s
```

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