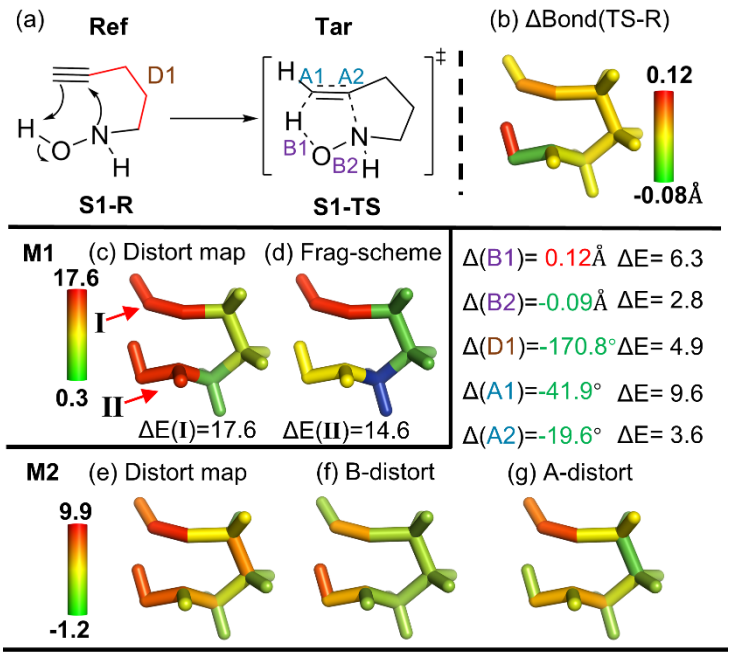
Tutorial for D2AF



Using the reverse Cope elimination as example

Structure file: Ref: 4F-reactant.gjf & **Tar**: TS-4F.gjf

4F-reactant.gjf contains the **connectivity** information

1. M1 scheme:

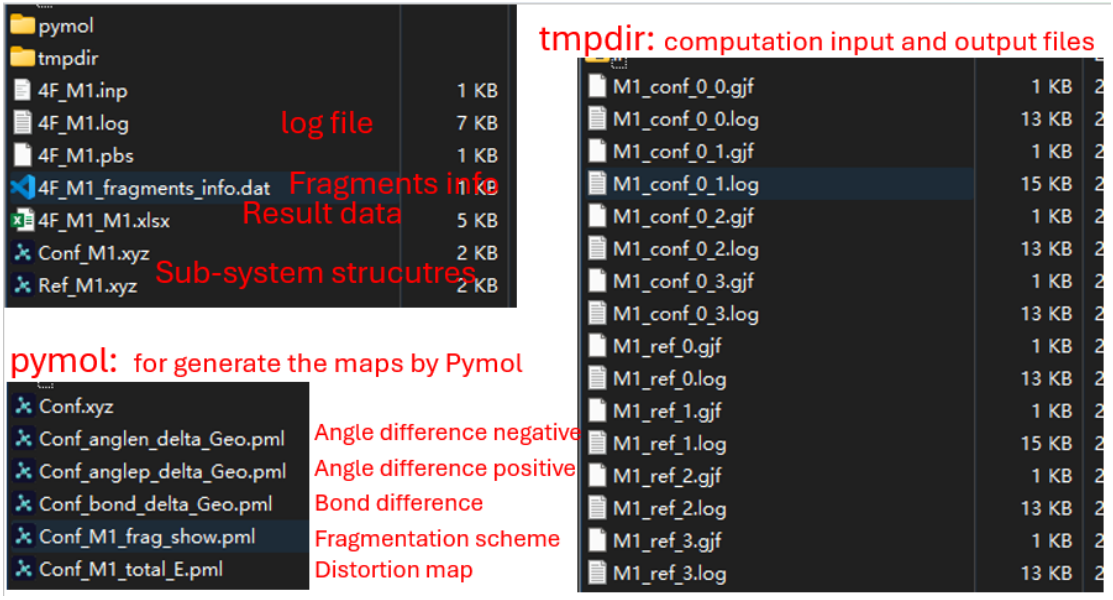
Input file: 4F_M1.inp

```
ref = 4F-reactant.gjf
conf = TS-4F.gjf
method = 1
cpu = 4
pal = 6
calculator = g16
scale=10

#fraglist
1,2,3
4-6,14-16
11-13
7-10
```

Pre-define the Gaussian 16 (or other calculators) environment then run:

D2AF -inp 4F_M1.inp > 4F_M1.log

Outputs as:



2. M2 scheme:

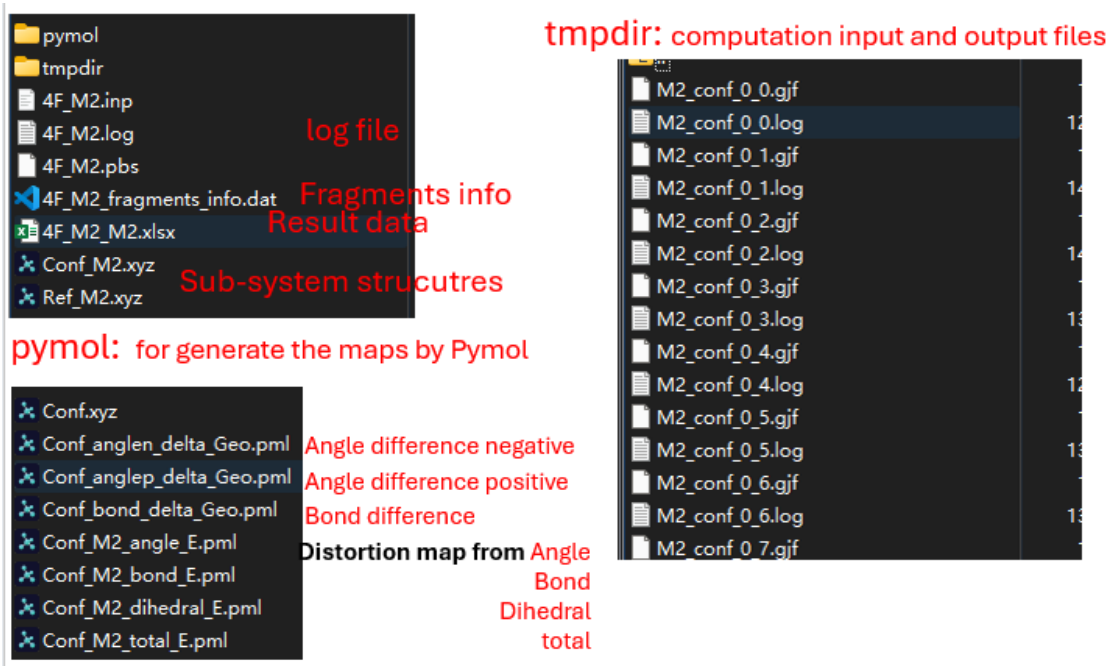
Input file: 4F_M2.inp

```
ref = 4F-reactant.gjf
conf = TS-4F.gjf
method = 2
cpu = 4
pal = 6
calculator = g16
scale=10

#include
1 4 14 11
```

Pre-define the Gaussian 16 (or other calculators) environment then run:

D2AF -inp 4F_M2.inp > 4F_M2.log

Outputs as:



3. M3 scheme:

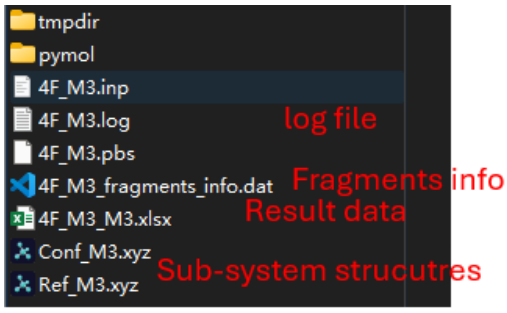
Input file: 4F_M3.inp

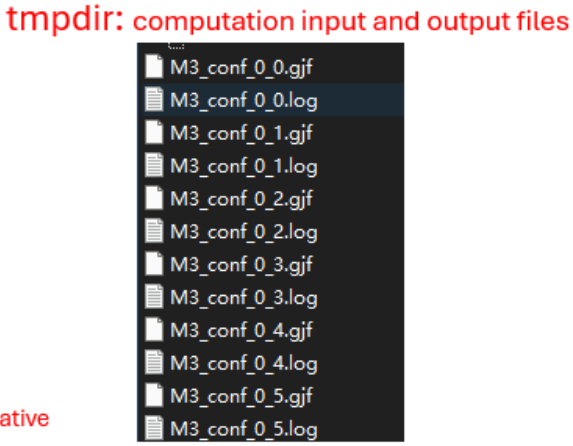
```
ref = 4F-reactant.gjf
conf = TS-4F.gjf
method = 3
cpu = 4
pal = 6
calculator = g16
scale=10

#fraglist
1,2,3

#include
1 4 14 11
```

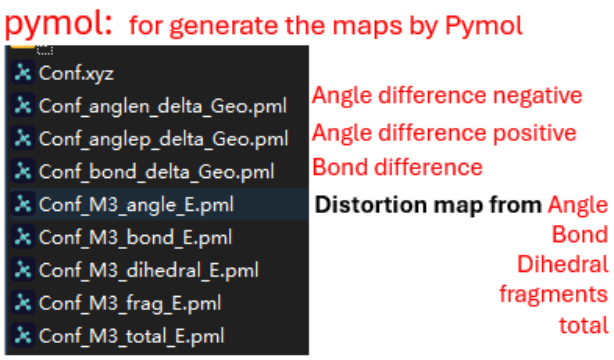
Pre-define the Gaussian 16 (or other calculators) environment then run:

D2AF -inp 4F_M3.inp > 4F_M3.log

Outputs as:







4. Energy computation by user (here use M2 as example)

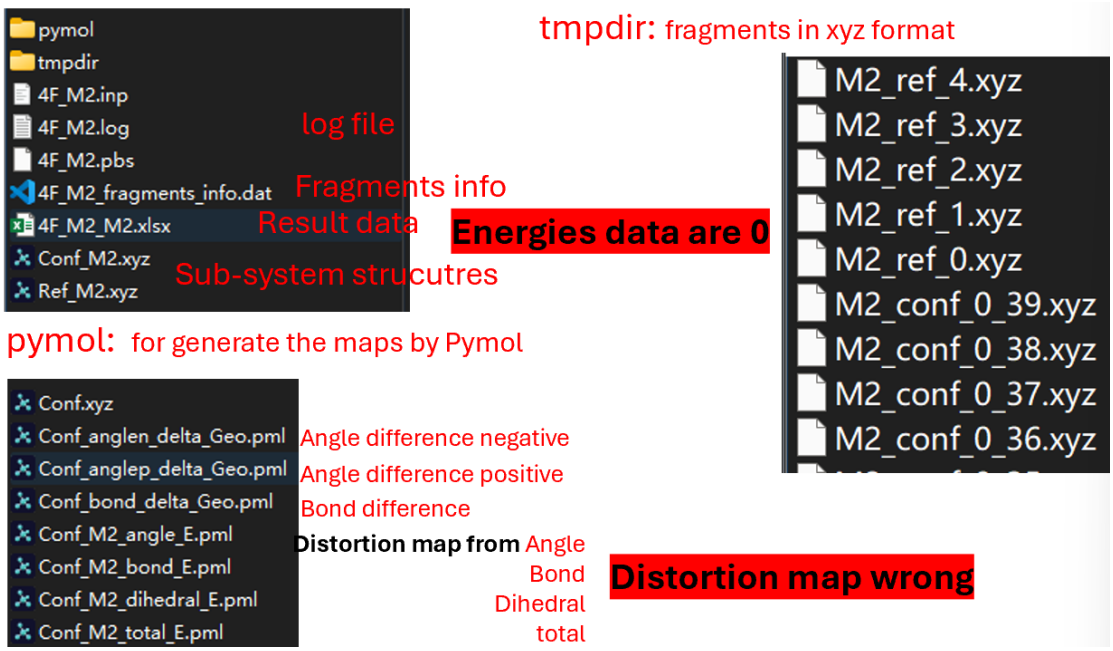
Input file: 4F_M2.inp

```
ref = 4F-reactant.gjf
conf = TS-4F.gjf
method = 2
cpu = 4
pal = 6
calculator = nocalc
scale=10

#include
1 4 14 11
```

run:

D2AF -inp 4F_M2.inp > 4F_M2.log

Outputs as:



Run QC calculations and extract the energies by users

Two possible ways to get the results (xlsx, pymol scripts for maps):

(a) Extract the energies to ****xxx_i.log**** *(in a.u. unit; 1st line) for each structure in the* ****\tmpdir**** *folder**

e.g.: **M2_ref_0.log** for **M2_ref_0.xyz**

-77.32558773

Run the following cmd again:

D2AF -inp 4F_M2.inp > 4F_M2.log

*(b) Extract the energies to a energy data file **M2_ene.dat***

Format of line (each line for one xyz file):

xyzname E(in a.u.)

```
M2_conf_0_0                -77.32041336
M2_conf_0_10               -172.06641049
M2_conf_0_11               -40.51684076
M2_conf_0_12               -79.82886505
M2_conf_0_13               -79.82882825
M2_conf_0_14               -131.69969592
M2_conf_0_15               -56.53531520
M2_conf_0_16               -95.83954060
M2_conf_0_17               -131.70256199
M2_conf_0_18               -171.01142018
```

Then run:

D2AF -d 4F_M2_M2.xlsx -m 2 -f pymol Conf.xyz -e M2_ene.dat

Strain energies in **4F_M2_M2.xlsx** and **pymol scripts** were updated based on **M2_ene.dat**

Output result is the same the **2. M2 scheme**

5. Others

Manual update xlsx data and regenerate maps

e.g.: exclude selected terms

or manual calculate the difference between the i^{th} ref and conf fragments and update the xlsx data

run:

D2AF -d 4F_M2_M2.xlsx -m 2 -f pymol Conf.xyz

pymol scripts were generated.

Output result is the same the **2. M2 scheme**