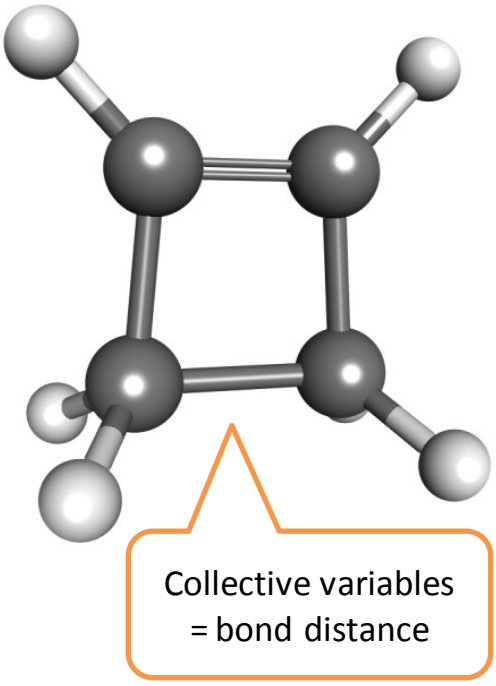
Metadynamics (MTD)

1. Calculation setup

The following setup is used.

- Method : MTD
- Potential : SMASH (b3lyp/cc-pvdz)
- System : C_4H_6 (cyclobutene)
- Maximum number of history-dependent Gaussian hills : 50000
- Gaussian hill height : 500 K
- Gaussian hill width : 0.1 bohr
- Mesh points of reconstructed hills potential : 1.0 bohr to 6.0 bohr with the increment of 0.02 bohr
- Collective variable : C-C bond distance

The reactant is shown below.



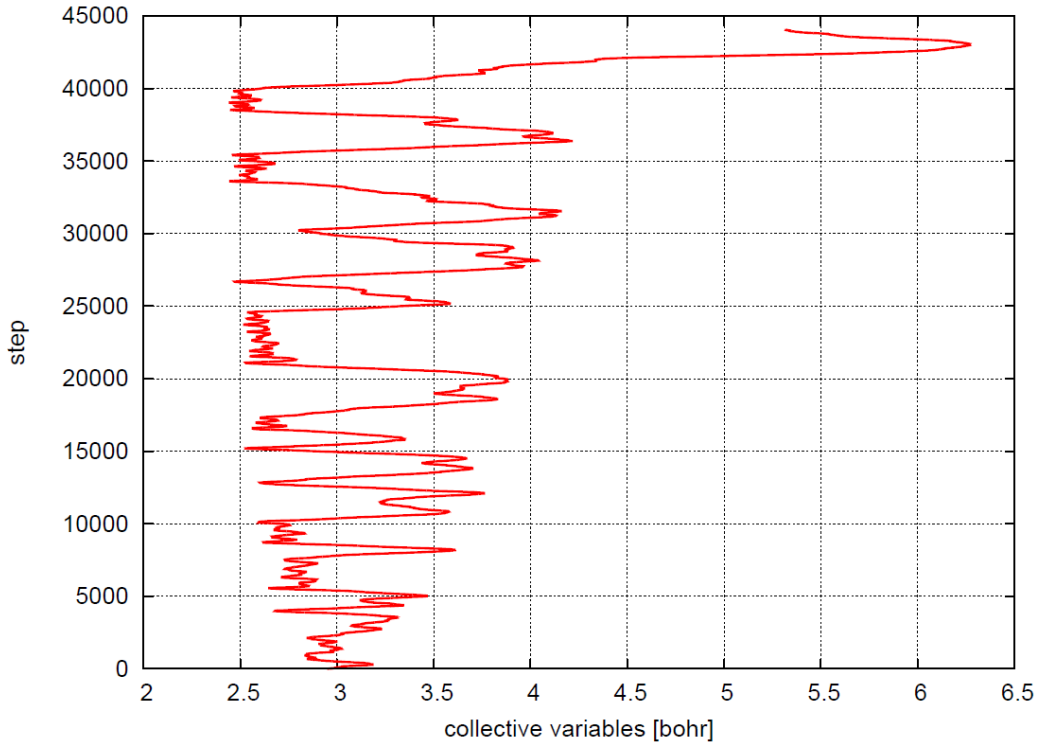
2. Results

The collective variable of each step is printed in “cv.out”.

step	rmeta	smeta
1	2.95056128	2.94965063
2	2.95134409	2.94985815
3	2.95209064	2.95062267
4	2.95280146	2.95194367
5	2.95349118	2.95359088
6	2.95418271	2.95522233
7	2.95489858	2.95653792
8	2.95565323	2.95738551
9	2.95644896	2.95778927
10	2.95727643	2.95792357

...omitted...

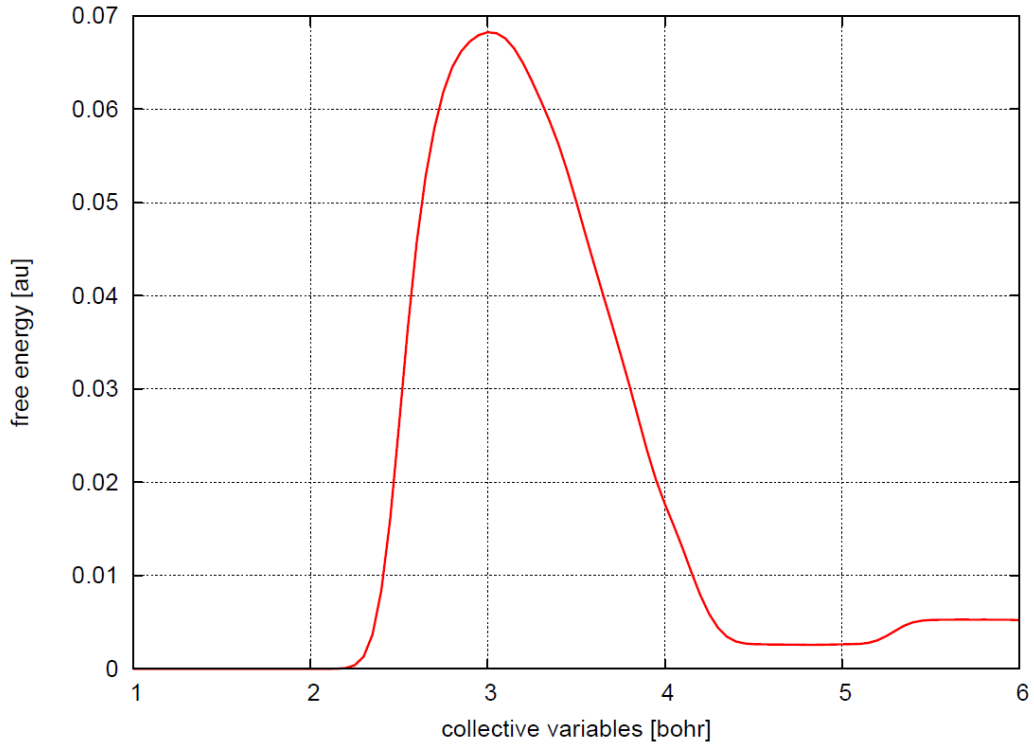
The collective variable (C–C distance) changes as below.



The free energy profile is printed in “rec.out”.

```
2.00000000     0.00000003
2.05000000     0.00000031
2.10000000     0.00000257
2.15000000     0.00001710
2.20000000     0.00009056
2.25000000     0.00038426
2.30000000     0.00131568
2.35000000     0.00366689
2.40000000     0.00840858
2.45000000     0.01607469
2.50000000     0.02604631
          ...omitted...
```

The free energy profile is plotted below.



The following structural change is found.