"coord.d" file is the only input file that users need to construct by themselves. The format should be the same as the instruction.

Coord.d (Example)

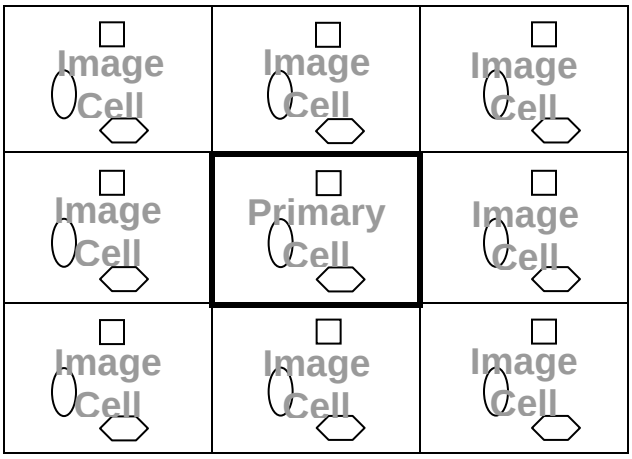
```
EQ of C60 w diamond terminated by H
1628
 0.00000000E+00
 0.17577400E+02   1.00000000E+15   0.17675300E+02
1       6      -8.364759   18.872859   -8.206983    1
2       6      -7.636139   18.357821   -6.94564     1
3       6      -8.364569   18.873015   -5.685102    1
 ⑦      ⑧           ⑨                      ⑩        ⑥
1626    1      6.924366    -19.984759  3.137823     1
1627    1      6.924557    -19.984602  5.659702     1
1628    1      6.924747    -19.984446  8.181583     1
1       0.000000    0.000000    0.000000
2       0.000000    0.000000    0.000000
3       0.000000    0.000000    0.000000
 ⋮        ⋮           ⋮           ⋮          ⑪
1626    0.000000    0.000000    0.000000
1627    0.000000    0.000000    0.000000
1628    0.000000    0.000000    0.000000
1       0.000000    0.000000    0.000000
2       0.000000    0.000000    0.000000
3       0.000000    0.000000    0.000000
 ⋮        ⋮           ⋮           ⋮          ⑫
1626    0.000000    0.000000    0.000000
1627    0.000000    0.000000    0.000000
1628    0.000000    0.000000    0.000000
1       0.000000    0.000000    0.000000
2       0.000000    0.000000    0.000000
3       0.000000    0.000000    0.000000
 ⋮        ⋮           ⋮           ⋮          ⑬
1626    0.000000    0.000000    0.000000
1627    0.000000    0.000000    0.000000
1628    0.000000    0.000000    0.000000
1       0.000000    0.000000    0.000000
2       0.000000    0.000000    0.000000
3       0.000000    0.000000    0.000000
 ⋮        ⋮           ⋮           ⋮          ⑭
1626    0.000000    0.000000    0.000000
1627    0.000000    0.000000    0.000000
1628    0.000000    0.000000    0.000000
```

① Comment line

② Total number of atoms in the system

③ Total elapsed time (fs): The total number of steps is 10,000 in the example input.d. So the total elapsed time will be 2,000 fs (= 10,000 x 0.2 fs) after one job.

④⑤ Size of the periodic boundary condition: It is very difficult to simulate more than a few million atoms at one time despite the advanced development of computing power in computers. In order to model a macroscopic system, the periodic boundary concept is often applied: The primary cell representing the bulk material is surrounded by image cells, images of the atoms in the primary cell. In this example coord.d, the dimension of the periodic boundary is 17.5774 (x) × :(= 1×10^{16}) (y) × 17.6753 (z) in (Å).



⑥ Position of Atoms

⑦ Atom number: There are 1628 atoms in this example.

⑧ Atomic number: These are defined in the input.d file. 6 is Carbon and 1 is Hydrogen.

⑨ Coordinates of atom: X, Y, and Z position of each atom

⑩ Type of atom (itr # or flag #): There are 4 types of atom as below

itr # or flag #	Description
0	Active (moving) atom. Movement due to the potentials between atoms.
1	Thermostats. Acts as if in a heat bath.
2	Fixed. Can't move.
3	Fixed and moving. Same as the fixed atom, however, movement of atom is possible if necessary by special, specific program.

⑪ 1st derivatives of the atom position in x, y, and z direction. (= velocity (Å/fs))

⑫ 2nd derivatives of the atom position in x, y, and z direction. (= acceleration)

⑬ 3rd derivatives of the atom position in x, y, and z direction.

⑭ 4th derivatives of the atom position in x, y, and z direction.

This is another file that C-H-O version REBO-MD code will read during the execution. This file is already hard copied in the interface. Users don't need to prepare this file. The instruction is just for user's information.

Input.d (Example)

```
-1 /thermostat
0.6955 0.500 /Random # seed, neighbor list
 1                          / =1 REBO (C,H,Si,Ge)
 1      1.0   15.0   2.81   / Hydrogen
 6     12.0   51.2   3.35   / Carbon Atom#,AtomM,eps(K),sigma(A) for LJ
-7     14.0   37.3   3.31   / Nitrogen
-8     16.0   80.5   3.03   / Oxygen
-60    12.0   28.1   2.76   / Carbon of Carbon Dioxide
-80    16.0   80.5   3.03   / Oxygen of Carbon Dioxide
-14    28.0   51.2   2.28   / Silicon = carbon
-10    20.0   47.0   2.72   / Neon
-18    40.0  119.8   3.41   / Argon
-36   131.0  164.0   3.83   / Krypton
```

①Thermostat: There are 4 thermostats. -1 represents the Langevin thermostat using frictional and random forces. 1 represents the Berendsen thermostat, 2 represents the zero velocity, and 3 represents Evan-Hoover thermostat. If unfamiliar with concept of thermostat, recommendation is to use –1.

②Random # seed: The seed number for the random function used in the calculation of the random force.

③Neighbor list: Parameter that controls neighbor list. Should not be changed from 0.500.

④Potential type: Use 1 when using REBO potentials.

⑤Atomic number: The program ignores the element having a negative sign (-) in front of the atomic number. 60 and 80 are used to distinguish the carbon and oxygen of carbon dioxide from normal carbon and oxygen

⑥Atomic weight (g/mol)

⑦Lennard-Jones parameter: ε (K). The Lennard-Jones potential is given by the expression

$$\varphi_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

⑧Lennard-Jones parameter: σ (Å)