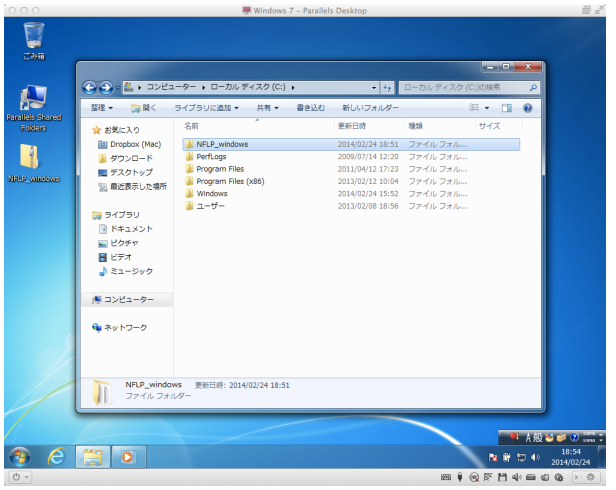
RMC tutorial

1．　Install WinNFLP

Unzip NFLP_windows.zip（extract to C:¥）



Contents of NFLP_windows folder

Calibration	NA
Correct	NA
Documentation	Documentation of RMCA etc.
Examples	Exapmles
Jmol-14.0.10	Jmol (visualize atomic configuration)
Rmc	executable code
Tables	
Templates	
UsefulAnalyzeCfg	Tools to analyze atomic configuration file
UsefulAnalyzeScfg	
UsefulCfg	Tools to create/modify configuration files
UsefulData	Tools to analyze RMC data
UsefulPlot	Tools to plot RMC data
readme.txt	
RMCA.ini	
WinNFLP.exe	GUI tools
WinNFLP.ini	

Jmol requires Java SE Development Kit 7

2．　Execute WinNFLP

Double click WinNFLP.exe in NFLP_windows folder

Dialog “Select Acrobat Reader”

Select Adobe Reader folder and “open” or “cancel”

Dialog “Select any file in desired working directory”

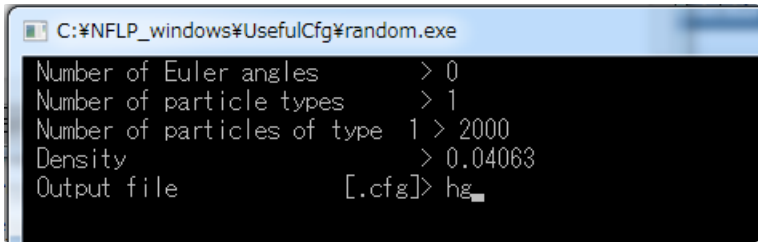
Select ▸NFLP_windows▸Examples▸RMCA_MCGR▸rmca_hg▸hg.dat and open

【Practice 1：model structure of liquid mercury】

- ✓ Model the structure of liquid mercury on the basis of x-ray $S(Q)$ by RMC.
- ✓ Create a random configuration, moveout closest atom, perform RMC, and analyze atomic configuration.
- ✓ Open ▸NFLP_windows▸Examples▸RMCA_MCGR▸rmca_hg folder to access files in the folder.
- ✓ It is better to set the environment of Windows to show extension of files.

3．　Create a random configuration

Execute Useful＞CFG programs＞Random




```
Number of Euler angles          > 0
Number of particle types        > 1
Number of particles of type 1   > 2000
Density                         > 0.04063
Output file              [.cfg] > hg
```

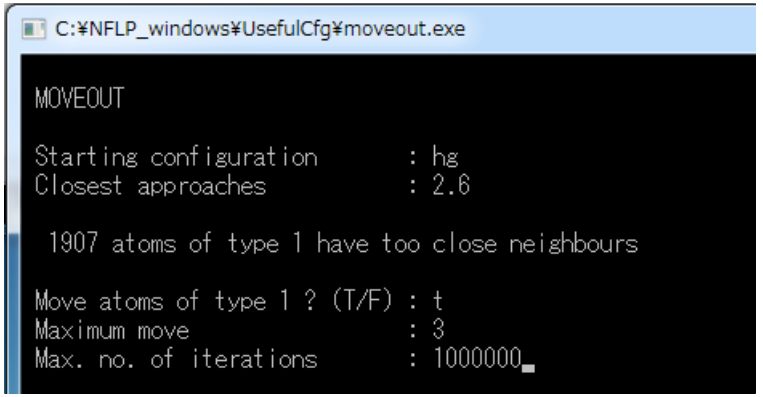
← single component system = 1

← atomic number density of mercury, / Å^3

← name of .cfg file

4. Moveout the atoms within closest approaches

Execute Useful＞CFG programs＞MoveOut




```
MOVEOUT
Starting configuration          : hg
Closest approaches              : 2.6
 1907 atoms of type 1 have too close neighbours
Move atoms of type 1 ? (T/F)    : t
Maximum move                    : 3
Max. no. of iterations          : 1000000
1907 atoms of type 1 have too close neighbours
after***** iterations
  . . . . . .
 364 atoms of type 1 have too close neighbours
after***** iterations
Continue ? (T/F)                : t
  . . . . . .
   0 atoms of type 1 have too close neighbours
after***** iterations
Re-calculate neighbours? (T/F) : f
Change cut-offs ? (T/F)         : f
Output file                     : hg
```

← file name of cfg file created by random

← 2.6 Å determined by experimental $g(r)$

← number of particle 1 which do not satisfy closest approaches

← move particle 1 or not?

← maximum distance (is necessary to change at random)

← repeat the process to reach 0 atoms by changing maximum move

← finish moveout

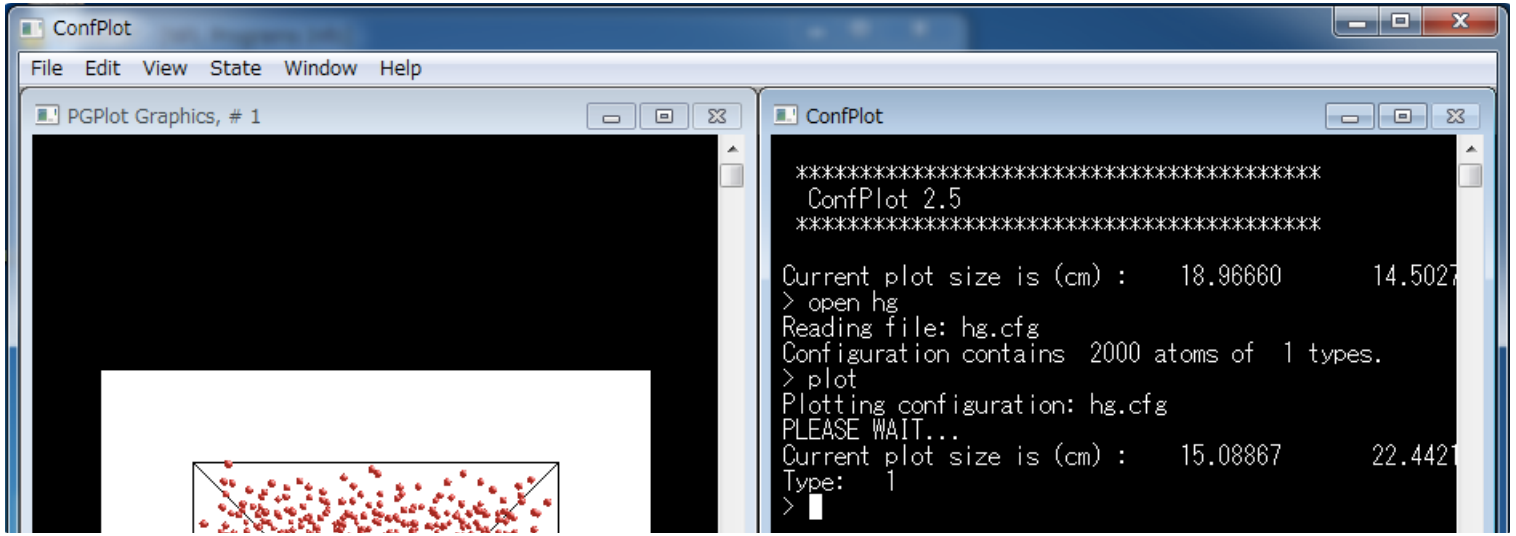
← don't re-calculate

← don't change cut-offs

← save file (overwrite)

5 . Visualization of atomic configuration

Execute Useful＞Plot programs＞ConfPlot




```
 ****************************************
  ConfPlot 2.5
 ****************************************
Current plot size is (cm) :    18.96660      14.50273
> open hg                                                    ← open “hg.cfg”
Reading file : hg.cfg
Configuration contains   200 atoms of  1 types.
> plot                                                       ← type “plot” for visualization
Plotting configuration: hg.cfg
PLEASE WAIT…
Current plot size is (cm) :    15.088672      22.442188
Type:   1
```

★ hg.cfg file（atomic configuration data）

```
(Version 3 format configuration file)                          ← title
Random configuration


        0        0        0 moves generated, tried, accepted   ← history of RMC
        0                  configurations saved

     2000 molecules (of all types)                             ← number of all particles
        1 types of molecule
        1 is the largest number of atoms in a molecule
        0 Euler angles are provided

        F (Box is not truncated octahedral)                    ← information of simulation box
          Defining vectors are:
           18.324457   0.000000   0.000000
            0.000000  18.324457   0.000000
            0.000000   0.000000  18.324457

     2000 molecules of type  1                                 ← side length of the simulation box
        1 atomic sites
           0.000000   0.000000   0.000000

-0.5556233 -0.7685104 -0.5371170                               ← fractional coordinates (x, y, z) -1 < xyz < 1
-0.8435115 -0.1586675 -0.9489551
 0.2504269 -0.2151476 -0.3068128
       . . . . . .
```

★ hg.dat（control file）

```
Liquid Hg@RT
0.04063                 ! number density
2.6
0.25                    ! maximum move
0 0.0                   ! nswap,swapfrac
0.05                    ! r spacing
.false.                 ! whether to use moveout option
0                       ! number of configurations to collect
9000 1                  ! step for printing,plotting
10 1                    ! Time limit, step for saving
0 1 0 0                 ! No. of g(r), neutron, X-ray, EXAFS expts
hgsq.dat
1 381                   ! Range of points used
1       ! Coefficients
3 0.01                  ! isig,Standard deviation
.false.
.false.                 ! whether to renormalize
1.0                     ! beta
.false.                 ! whether to offset
1                       ! nback
0.                      ! bcoeff
.false.
0                       ! no. of coordination constraints
0                       ! no. of average coordination constraints
0                       ! no. of bvs constraints
0                       ! no. of triplet constraints
.false.                 ! whether to use a potential
```

← title
← number density Å^3
← closest distance
← maximum movement
← r step
← number of experimental data
← file name of x-ray $S(Q)$

6．　Final RMC modeling with x-ray $S(Q)$

Execute Rmc＞RMCA

Dialog　“Select a file” , open hg.dat

Then RMC will be automatically initialized

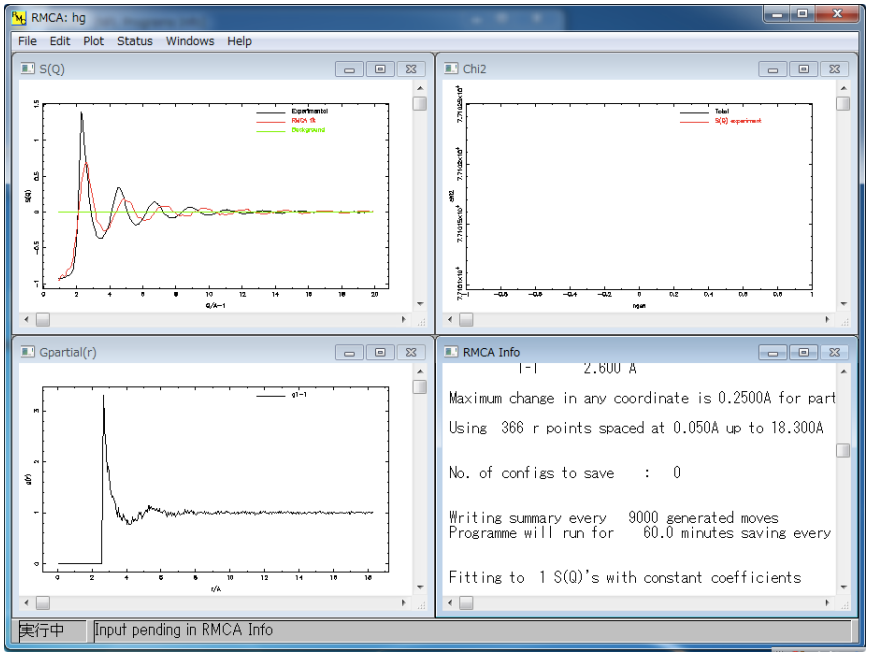
・$S(Q)$　　Black: experimental X-ray $S(Q)$

Red: calculated $S(Q)$ by RMC

・Chi2　　Black: total　χ^2

Red:　χ^2 of $S(Q)$

・Gpartial(r)　　Black: Partial $g(r)$



・RMCA Info window

Scroll down the window and you will find

`Begin (Y/N)?`

Type “y” for start of RMC

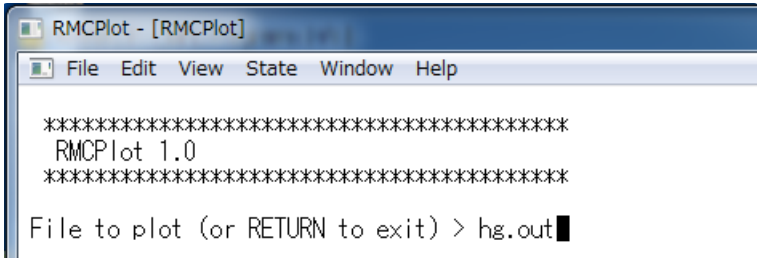
To control RMC run

Status＞Pause（Ctrl+S）	Pause RMC
Status＞Resume（Ctrl+Q）	Repause RMC
File＞Save	Save the results of RMC
File＞Exit	Quit RMC

✓　*I*t is necessary to run to converge the　χ^2

7 . To plot the results of RMC

Execute Useful＞Plot programs＞RMCPlot




```
*****************************************
 RMCPlot 1.0
*****************************************
File to plot (or RETURN to exit) > hg.out
Input file contains   3 groups of plots:
  Group   1 contains   1 plots of  1 curves
  Group   2 contains   1 plots of  1 curves
  Group   3 contains   1 plots of  2 curves
Plot which group (enter 0 to exit) ? 1
Change limits ? (T/F) > t
Data limits are             :
 5.0000001E-02     18.30000          0.0000000E+00
2.913868
Current plotting limits are :
 -0.8625000            19.21250        -0.1456934
3.59561
Enter new limits > 0 20 0 3
```

← "hg.out" contains $g(r)$ and $S(Q)$ calculated by RMC together with experimental data

← Group 1 : partial $g_{ij}(r)$

← Group 2 : partial $S_{ij}(Q)$

← Group 3 : $S(Q)$s

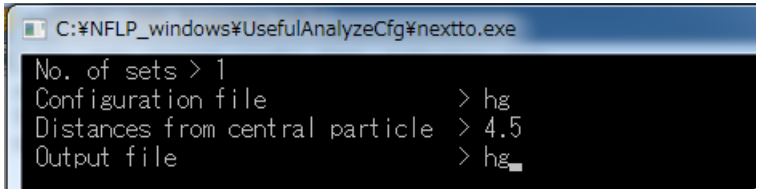
← Select Group 1

← to change X axis : 0～20, Y axis : 0～3

✓ It is necessary to make dure the first coordination distance in $g_{ij}(r)$, which should be found at around 4.5Å

8. Calculation of the distribution of coordination number

Execute Useful＞Analyze CFG programs＞NextTo

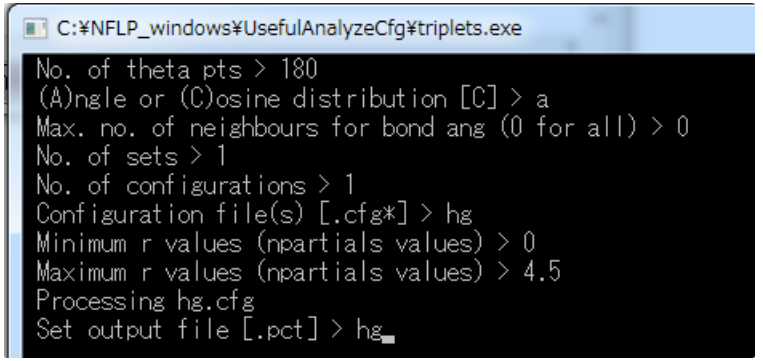



```
No. of sets > 1
Configuration file                      > hg          ← select hg.cfg
Distances from central particle         > 4.5         ← input the first coordination distance
Output file                             > hg          ← output to “hg.nei”
```

✓ Open hg.nei by text editor to see the distribution of coordination number of Hg around Hg within 4.5 Å

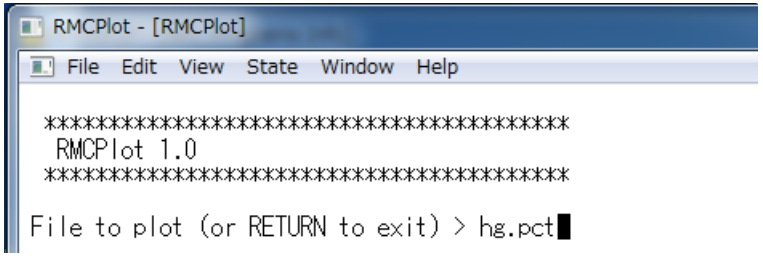
9. Calculation of Hg-Hg-Hg triplet angle

Execute Useful＞Analyze CFG programs＞Triplets




```
No. of theta pts > 180
(A)ngle or (C)osine distribution [C] > a          ← Angle or Cosine
Max. no. of neighbours for bond ang (0 for all) > 0
No. of sets > 1
No. of configurations > 1
Configuration file(s) [.cfg*] > hg                ← input the file name of .cfg
Minimum r values (npartial values) > 0
Maximum r values (npartial values) > 4.5
Processing hg.cfg
Set output file [.pct] > hg
```

Execute Useful＞Plot programs＞RMCPlot




```
 ****************************************
  RMCPlot 1.0
 ****************************************
File to plot (or RETURN to exit) > hg.pct          ← select “hg.pct”
Change limits ? (T/F) > t                          ← change plot range
Data limits are             :
  173.9578    6.042285   0.0000000E+00  0.8882140
Current plotting limits are :
 -2.353492    182.3536  -4.4410702E-02  0.9326247
Enter new limits > 0 180 0 1                       ← change x-axis：0～180、y-axis：0～1
```

【Practice 2：model the structure of SiO_2 glass】

Preparation

Execute WinNFLP.exe

Dialog “Select any file in desired working directory

Select ▸NFLP_windows▸Examples▸RMCA_MCGR▸rmca_sio2▸sio2.dat

- ✓ Model the structure of SiO_2glass by using a combination of neutron $S(Q)$ and x-ray $F(Q)$
- ✓ The order is Random, MoveOut, Hard Sphere Monte Carlo (HSMC) simulation to create a Q^4 network, RMC simulation, and analysis of RMC configuration.

1． Create a random configuration

Execute Useful＞CFG programs＞Random

```
Number of Euler angles          > 0
Number of particle types        > 2
Number of particles of type 1   > 550
Number of particles of type 1   > 1100
Density                         > 0.06615

Output file              [.cfg] > sio2
```

← 2 atomic type, Si and O
← number of Si atom: 550
O atom: 1100
←atomic number density of SiO_2 ($Å^{-3}$) which can be calculated by a mass density

2．　Moveout the atoms within closest approaches

Execute Useful＞CFG programs＞MoveOut

```
MOVEOUT
Starting configuration          : sio2              ← input the file name of initial configuration created by random
Closest approaches              : 2.9 1.5 2.4       ← closest distance for Si-Si, Si-O, and O-O
  524 atoms of types1 have too close neighbours
 1037 atoms of types2 have too close neighbours
Move atoms of type 1 ? (T/F)    : t                 ← move type 1 (Si)
Move atoms of type 2 ? (T/F)    : t                 ← move type 2 (O)
Maximum move                    : 3                 ← distance for maximum move
Max. no. of iterations          : 1000000
   ・・・(省略)・・・
   0 atoms of types1 have too close neighbours
after***** iterations
Re-calsulate neighbours? (T/F) : f
Change cut-offs ? (T/F)         : f
Output file                     : sio2
```

3．　Perform Hard Sphere Mote Carlo (HSMC) simulation (RMC w/o experimental data) and RMC simulation

	Constraints	experimental data	Coordination number (CN) constraints	Where in .dat file
(1)	Neutron $S(Q)$	siogemsq.dat		line 13～23
(2)	X-ray $S(Q)$	sio04sq.dat		line 24～33
(3)	Four fold Si		CN of O around Si in $0 < r < 1.8$Å should be 4	line 35
(4)	Two fold O		CN of Si around O in $0 < r < 1.8$Å should be 2	line 36
(5)	zero fold Si (optional)		CN of O around Si in $1.8 < r < 2.2$Å should be 0	line 37

It is important point that we need preliminary HSMC run to create Q4 network by interconnestion of SiO4 tetrahedra with sharing oxygen at the corner before final RMC run with both neutron and x-ray $S(Q)$. In HSMC run, we use only constraints (3) and (4) in the table above.

- ✓ Copy original "sio2.dat" to "sio2.dat_orig".
- ✓ Open "sio2.dat" by a text editor
  - Modify the description of experimental data in line 12 `0 1 1 0` → `0 0 0 0`
  - Delete the description for neutron $S(Q)$ in line 13～23
  - Delete the description for x-ray $F(Q)$ in line 24～33
  - Modify the description for CN constraints in line 34 `3` → `2`
  - Delete the description for CN constraints in line 37

```
SiO2 network (hard sphere MC)
0.06615                 ! number density
2.90 1.50
    2.45                ! cut offs
0.25 0.25               ! maximum move
0 0.0           ! nswap,swapfrac
0.05            ! r spacing
.false.                 ! whether to use moveout option
0                       ! number of configurations to collect
9000 1                  ! step for printing,plotting
60 10                   ! Time limit, step for saving
0 0 0 0                 ! No. of g(r), neutron, X-ray, EXAFS expts      ← no experimental data in a HSMC run
2                       ! no. of coordination constraints               ← modify the number of CN constraints
1 2 0.  1.8  4 1. 0.00001                                               ← CN of O around Si in 0～1.8Å should be 4
2 1 0.  1.8  2 1. 0.00001                                               ← CN of Si around O in 0～1.8Å should be 2
0                       ! no. of average coordination constraints
0                       ! no. of bvs constraints
0                       ! no. of triplet constraints
.false.                 ! whether to use a potential
```

To start a HSMC run,

Exectute Rmc＞RMCA

Dialog “Select a file” , open sio2.dat

In “RMCA Info” window

Scroll down the window and you will find

```
Begin (Y/N)?
```

Type “y” for start of final RMC run

It will take time to satisfy coordination number constraints (to be explained in detail in tutorial).

4. Final RMC run

Preparation

Delete “sio2.dat” and rename “sio2.dat_orig” to “sio2.dat”

5. To plot the results of RMC run

Execute Useful＞Plot programs＞RMCPlot and plot “sio2.out”

✓ It is necessary to make sure the first coordination distance for Si-Si, Si-O, and O-O which should be found at around 3.5, 1.8, and 3.0Å, respectively.

To visualize atomic configuration, execute Useful＞Plot programs＞ConfPlot

To bond Si and O by a line,

```
> bond 1 2 0 1.8
> plot
```

6．　配位数分布の解析

Useful＞Analyze CFG programs＞NextTo を起動します。

```
No. of sets > 1
Configuration file                    > sio2
Distances from central particle       > 1.8 1.8
Output file                           > sio2        ← output to “sio2.nei”
```

7．　Analysis of bond angle distributions

Execute Useful＞Analyze CFG programs＞Triplets

```
No. of theta pts > 180
(A)ngle or (C)osine distribution [C] > a
Max. no. of neighbours for bond ang (0 for all) > 0
No. of sets > 1
No. of configurations > 1                          ← number of configuration (should be 1)
Configuration file(s) [.cfg*] > sio2
Minimum r values (npartial values) > 0 0 0         ← minimum distance for Si-Si, Si-O, and O-O pairs
Maximum r values (npartial values) > 3.5 1.8 3.0   ← maximum distance for Si-Si, Si-O, and O-O pairs
Processing sio2.cfg
Set output file [.pct] > sio2                      ← fine name for output
```

✓　To plot bond angle distributions

Execute Useful＞Plot programs＞RMCPlot

```
File to plot (or RETURN to exit) > sio2.pct        ←select sio2.pct
```

Upper : Si-Si-Si、Si-Si-O、O-Si-O
Lower : Si-O-Si、Si-O-O、O-O-O

8．　Analysis of ring statistics

Execute Useful＞Analyze CFG programs＞Rings

```
Configuration file [.cfg] > sio2
Binary network ? [T/F] > t
Which types > 1 2                                  ← type 1(Si) and type 2 (O)
Output file name [.rng] > sio2                     ← output file name is “sio2.rng”
Maximum ring size > 12                             ← maximum size of ring is set to 12
Maximum distance between neighbours > 1.8          ← first coordination distance for Si-O is 1.8 Å
Detailed statistics output y/[n]? > y              ← name of output file is “sio2.rst”
```

9. Convert .cfg file to a RasMol file

Execute Useful＞Plot programs＞RasMolConv

```
Enter input file name  [.cfg] > sio2
Enter label for type  1 : Si
Enter label for type  2 : O
Enter output file name [.xyz] > sio2
```

✓ To plot .xyz file by Jmol

Excecute Jmol and open “sio2.xyz.