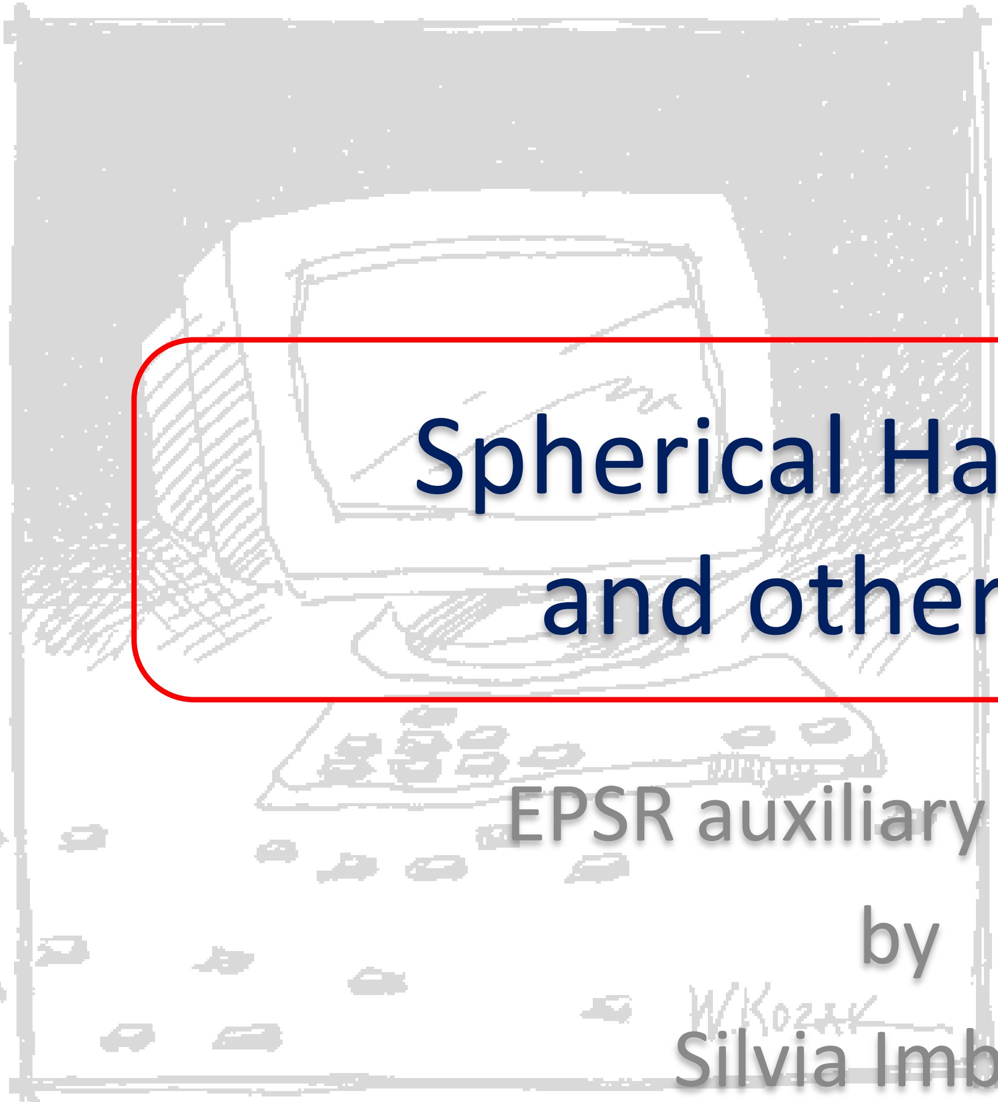

Spherical Harmonics and other tales

EPSR auxiliary routines

by

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ISIS

Operative flowchart

Setup EPSR simulation

Run EPSR simulation (3 steps):

- MC with Reference Potential (without any input from the data)
- Potential Refinement (MC loop with potential adjustment)
- Accumulation of Configurations (in this phase we keep refining the potential)

Analysis of the configurations accumulated

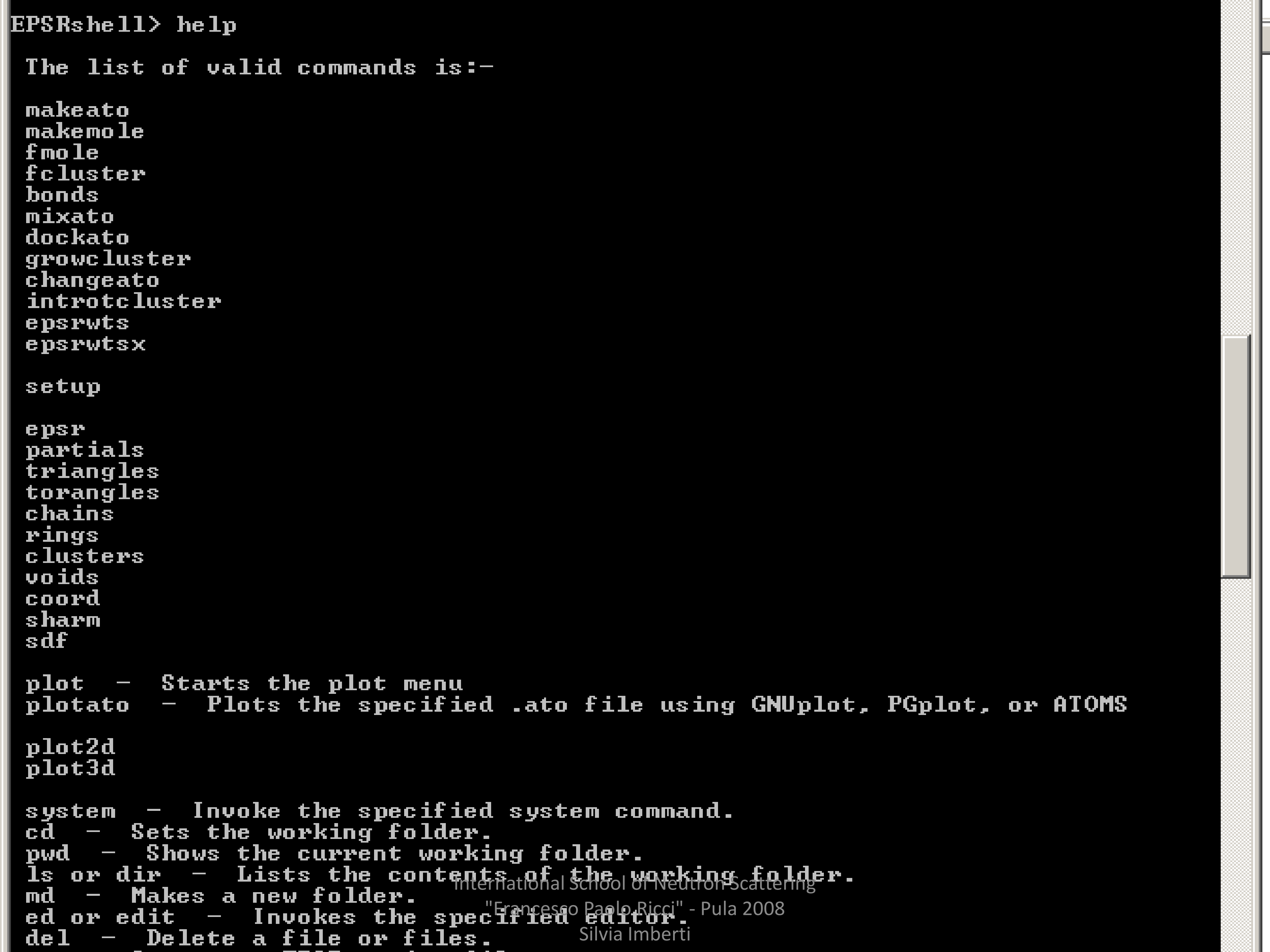
6. Auxiliary routines.

6.1. Input and output data formats and running.
6.2. **partials** – calculate site-site radial distribution functions. (obsolete)
6.3. **coord** – calculate coordination numbers and coordination number distributions about specific sites.
6.4. **triangles** – calculate bond angle distribution functions.
6.5. **torangles** – calculate torsional angle distribution functions.
6.6. **clusters** – calculate cluster size distribution functions.
6.7. **chains** – calculate chain length distribution functions.

6.8. **rings** – calculate ring length distribution functions.

7. Spherical harmonic expansion of many-body correlation functions.

7.1. Introduction – the spatial density function and orientational correlation function
7.2. **sharm** – calculates the spherical harmonic coefficients for the spatial density function and orientational pair correlation function
7.3. **sdf** – spatial density functions for non-molecular systems.
7.4. **plot2d** and **plot3d** – plotting the results from 7.2 and 7.3.
7.5. Triple body correlation function and higher order correlation functions.



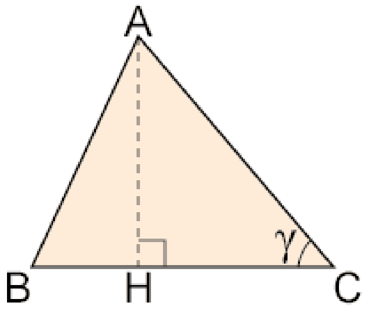
```
EPSRshell> help

 The list of valid commands is:-

 makeato
 makemole
 fmole
 fcluster
 bonds
 mixato
 dockato
 growcluster
 changeato
 introtcluster
 epsrwts
 epsrwtsx

 setup

 epsr
 partials
 triangles
 torangles
 chains
 rings
 clusters
 voids
 coord
 sharm
 sdf

 plot  -  Starts the plot menu
 plotato  -  Plots the specified .ato file using GNUplot, PGplot, or ATOMS

 plot2d
 plot3d

 system  -  Invoke the specified system command.
 cd  -  Sets the working folder.
 pwd  -  Shows the current working folder.
 ls or dir  -  Lists the contents of the working folder.
 md  -  Makes a new folder.
 ed or edit  -  Invokes the specified editor.
 del  -  Delete a file or files.
```

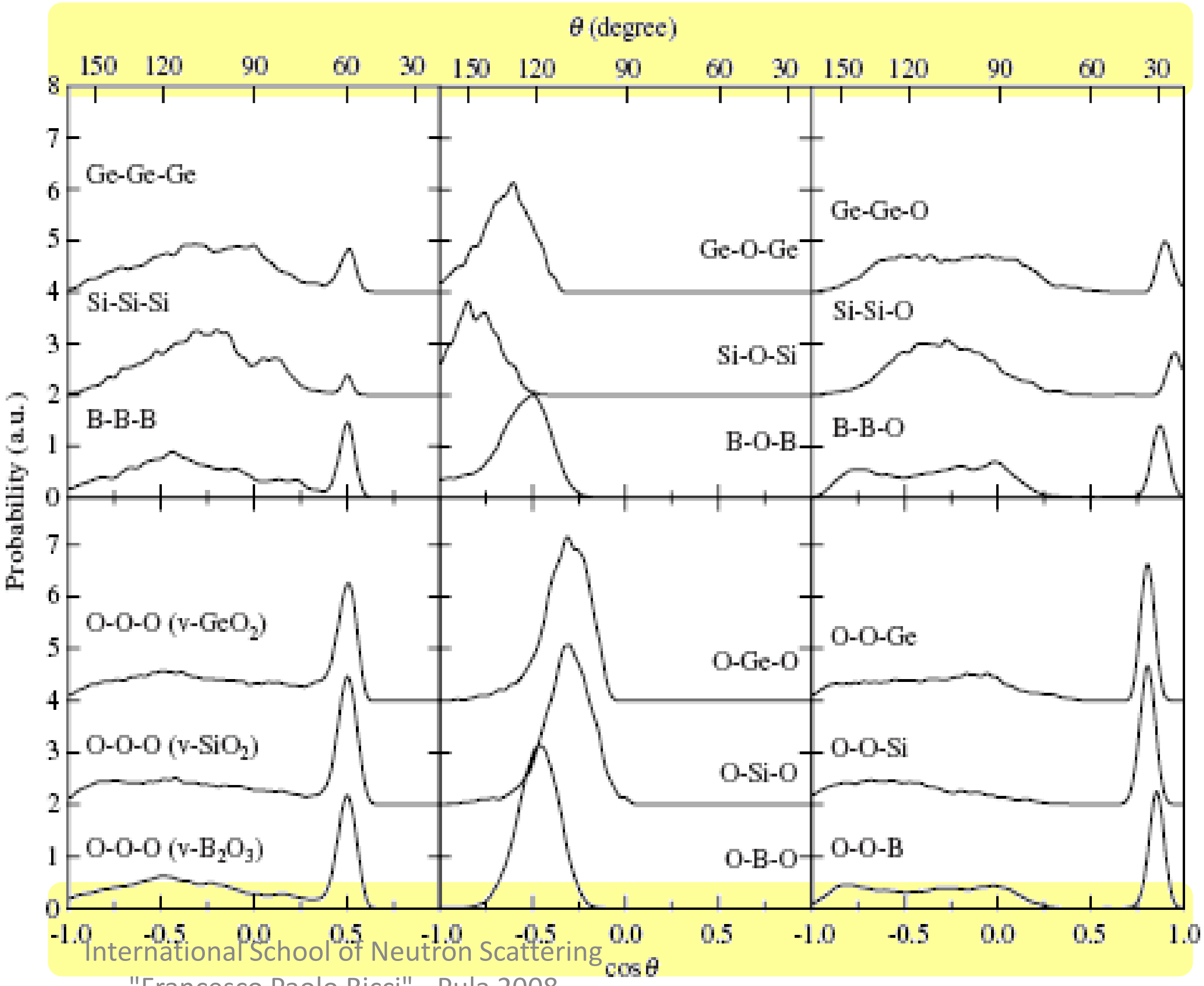
Basic	What for	How to (theory)	How to (practice)
Triangles calculates the distribution of angles between three atoms which satisfy the specified distance constraints	The importance of correcting for the solid angle sampling (SiO2)	Analytical geometry (from the set of coordinates)	•Setup **<program>** <input filename.dat> • Input and Output files format • Commands that can be run either as one-offs or repeatedly in a script file • Plot routines

The importance of correcting for the solid angle sampling

Carnot's theorem

$$\overline{AB}^2 = \overline{AC}^2 + \overline{BC}^2 - 2\overline{AC} \cdot \overline{BC} \cos\gamma$$

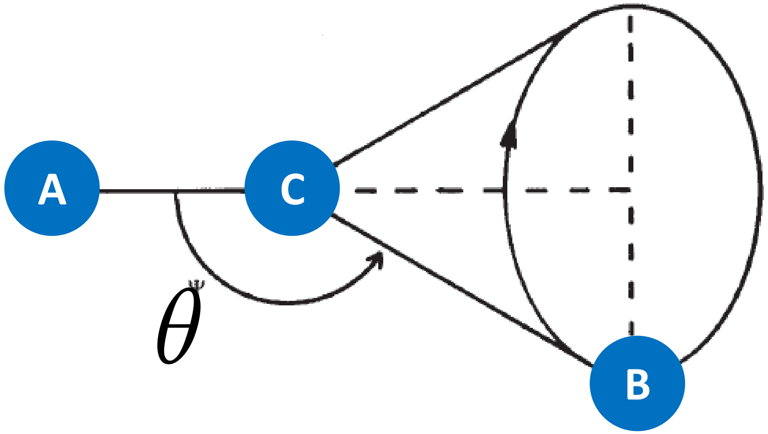




Since the cosine is a non-linear function, equal spacing in cosine doesn't correspond to equal spacing in the actual bond angle

Do you think this plot is correct?

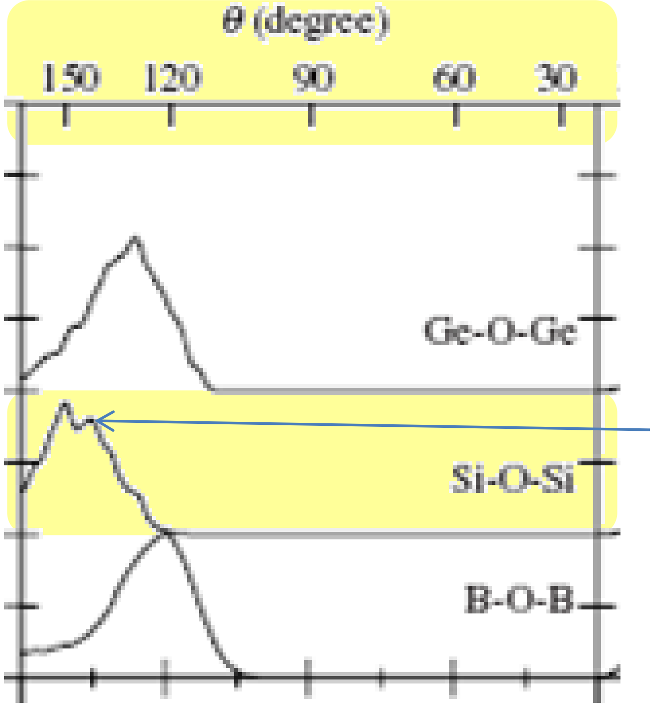
Whenever we make a variable transformation we have to correct the dependent variable for the so-called Jacobian…



This is in fact taking into account that I have more possibilities for atom B to lie at an angle of say 45º than 20º

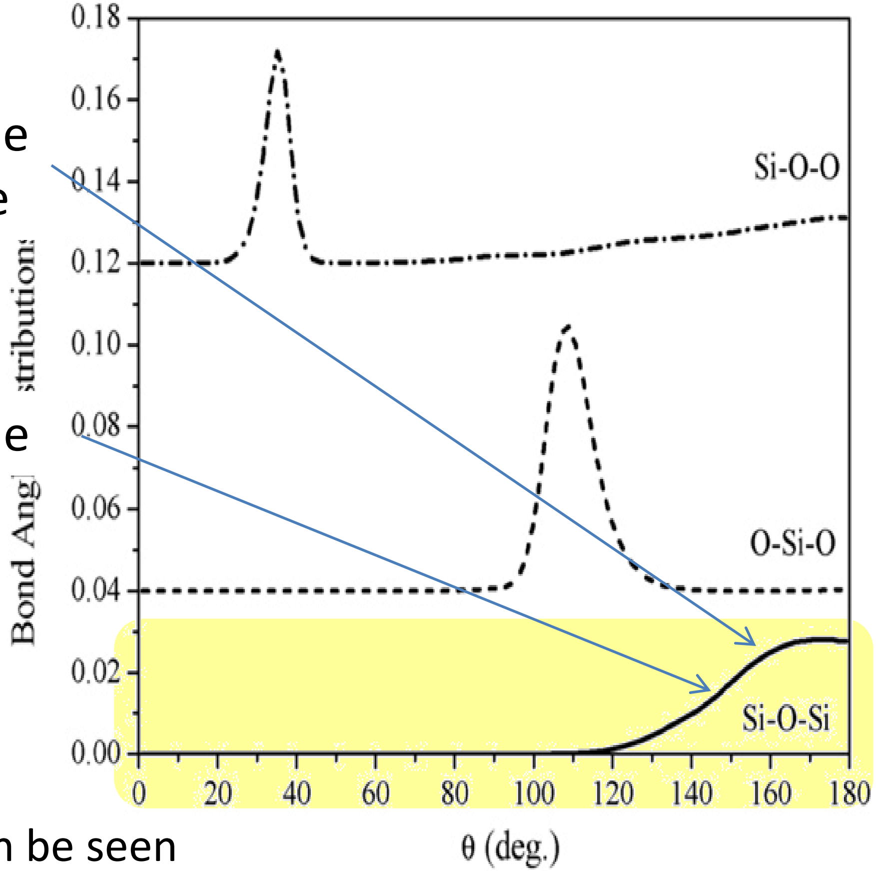
$$f(\cos(\theta))d\cos(\theta) = f(\cos(\theta))\frac{d\cos(\theta)}{d\theta}d\theta$$

$$f(\cos(\theta))d\cos(\theta) = g(\theta)\sin(\theta)d\theta$$

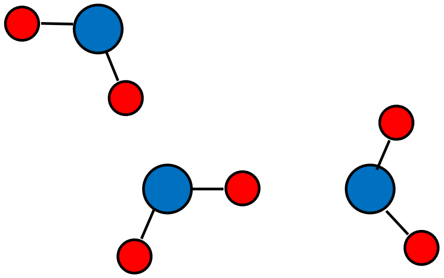


Most probable (modal) angle

Average angle



The Si–O–Si bond angle distribution function can be seen to have a modal value close to a linear bond i.e., 180◦.

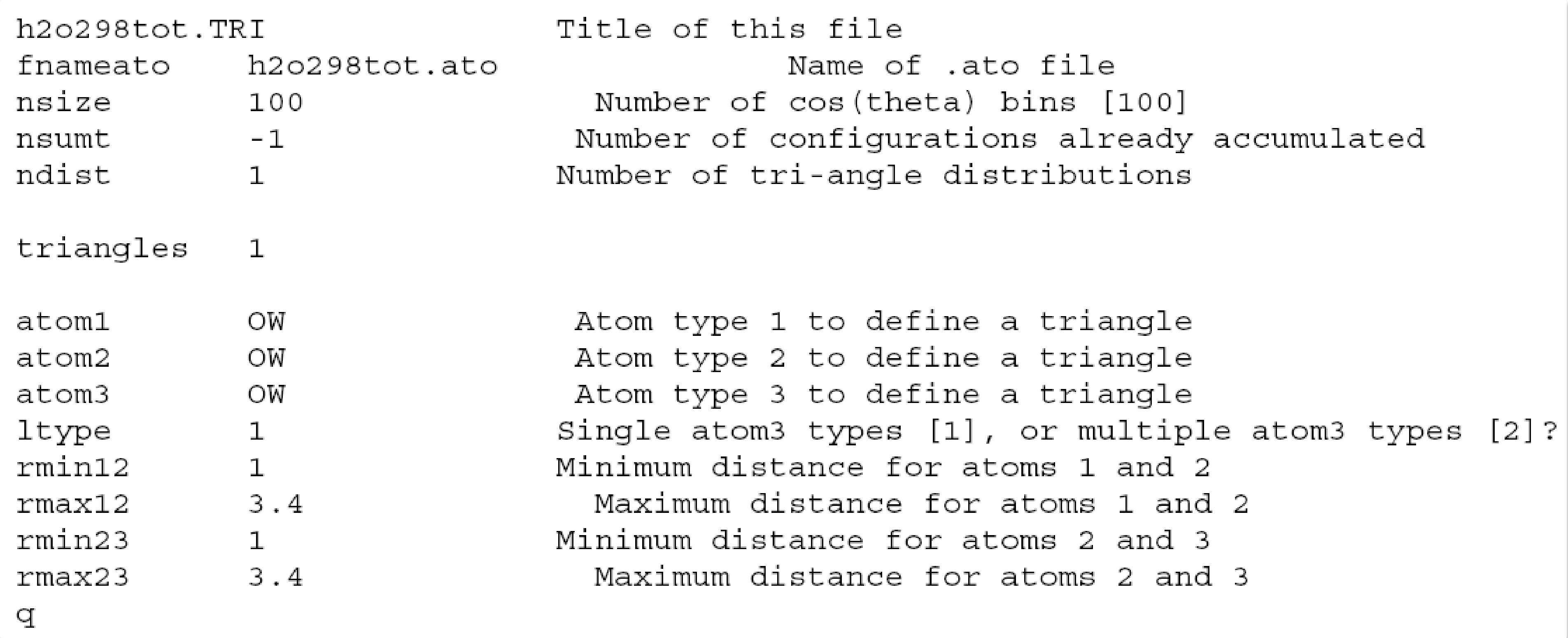


The combination of
- •*Si–O* coordination number = 3.9 oxygen atoms around each silicon atom
- •dominant 109◦ O–Si–O and 35◦ Si–O–O bond angles confirms the basic tetrahedral structure of this glass.

D.T. Bowron / Materials Science and Engineering B 149 (2008) 166–170

Input file for TRIANGLES
(either with “setup” from the shell of copying and modifying an example file)

<filename>.TRI.dat



```
h2o298tot.TRI               Title of this file
fnameato    h2o298tot.ato               Name of .ato file
nsize       100               Number of cos(theta) bins [100]
nsumt       -1               Number of configurations already accumulated
ndist       1               Number of tri-angle distributions

triangles   1

atom1       OW               Atom type 1 to define a triangle
atom2       OW               Atom type 2 to define a triangle
atom3       OW               Atom type 3 to define a triangle
ltype       1               Single atom3 types [1], or multiple atom3 types [2]?
rmin12      1               Minimum distance for atoms 1 and 2
rmax12      3.4               Maximum distance for atoms 1 and 2
rmin23      1               Minimum distance for atoms 2 and 3
rmax23      3.4               Maximum distance for atoms 2 and 3
q
```

Output files (very general)

As a general rule the input and output files for EPSR and its auxiliary routines will have a double extension of the form

<filename>**.<program>**.<filetype>

.TRI	triangles input and output files
.TOR	torangles input and output files
.CLUSTERS	clusters input and output files
.CHAINS	chains input and output files
.RINGS	rings input and output files
.SHARM	sharm input and output files
.SDF	sdf input and output files

<filename>.<program>**.<filetype>**

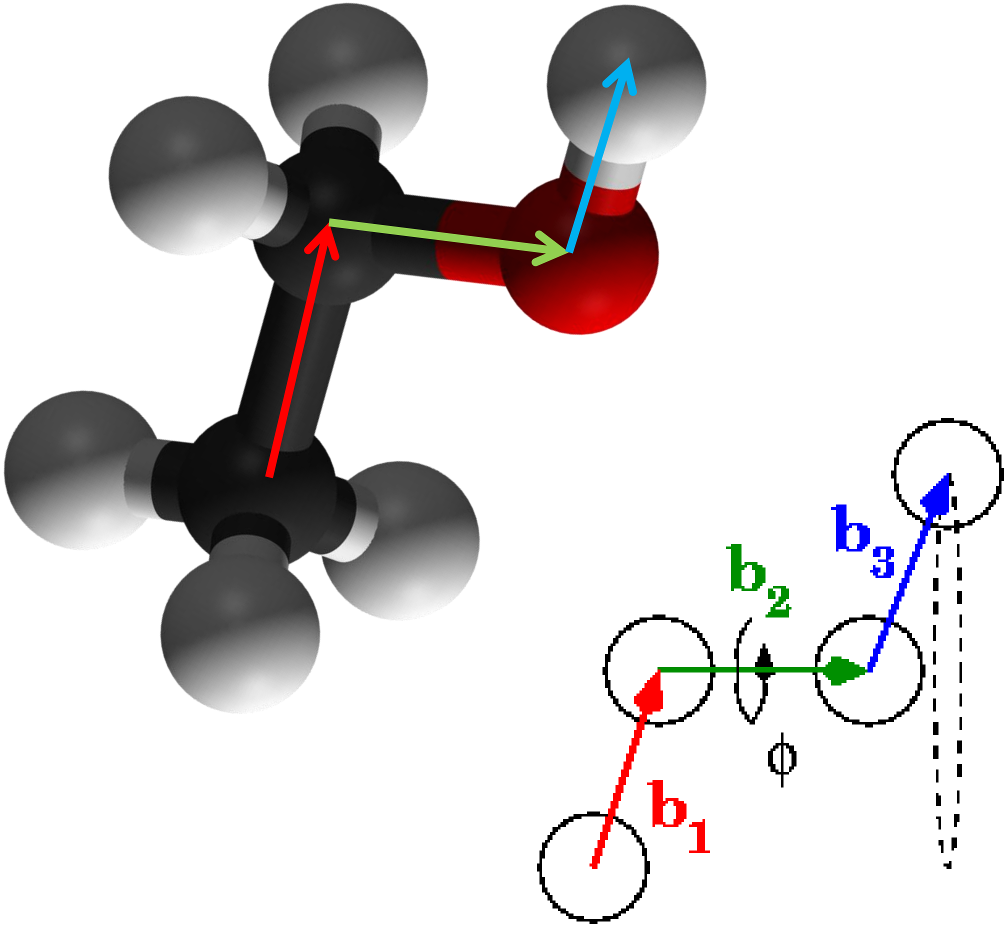
.c01	output files for TRIANGLES and TORANGLES angle distributions
.n01	output files for CLUSTERS, CHAINS, COORD, RINGS distribution functions
.h01, .h02, etc.	output files for SHARM and SDF coefficients

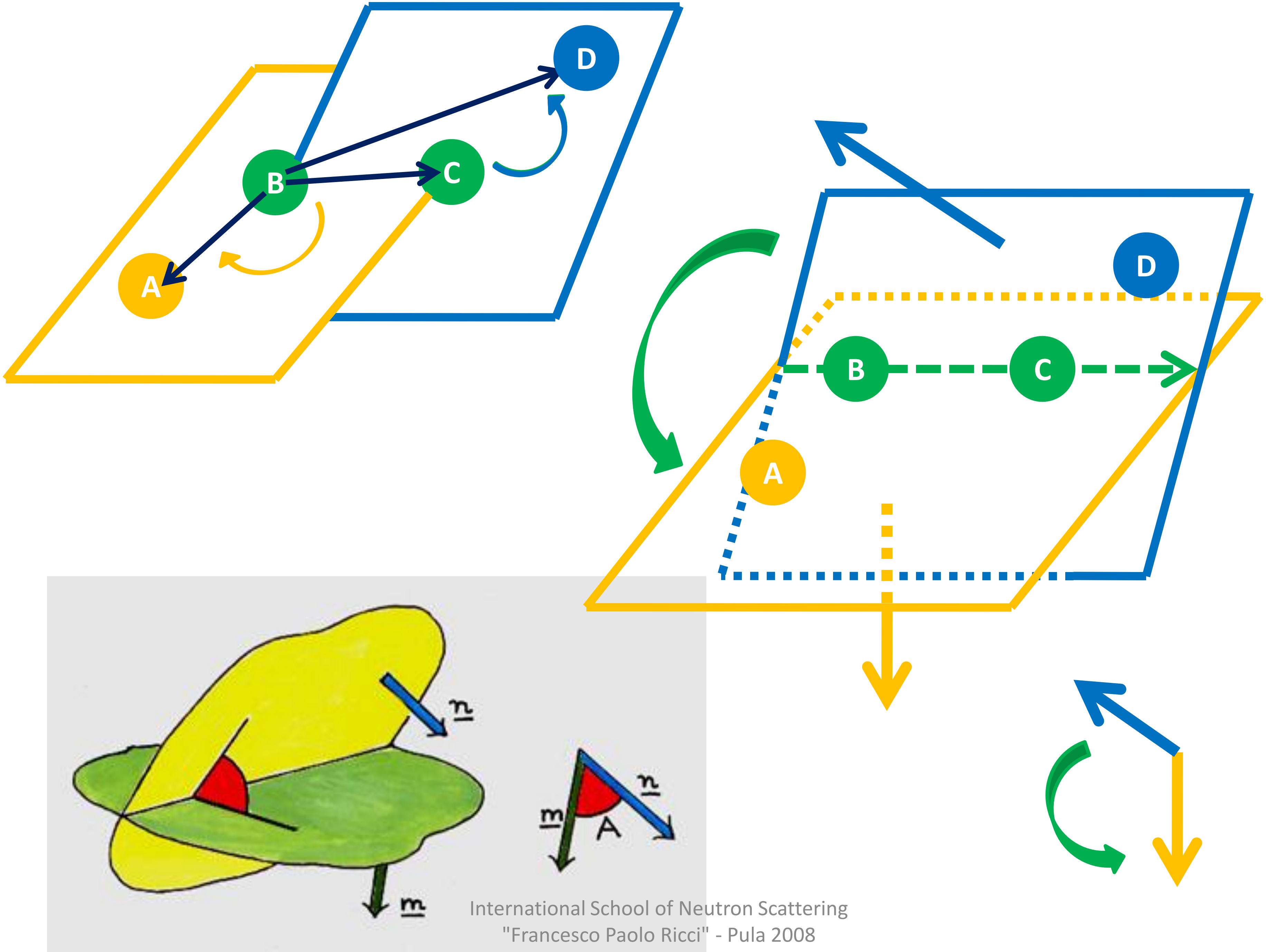
# Basic	What for	How to (theory)	How to (practice)
Triangles		Analytical geometry (from the set of coordinates)	• Setup **<program>** <filename>.<program>.dat • Input and Output files format • Commands that can be run either as one-offs or repeatedly in a script file • Plot routines
Torangles calculates the distribution of angles between four atoms (aka torsion or dihedral angle)			

The analytical geometry bit

The dihedral or torsion angle of two planes can be seen by looking at the planes "edge on", i.e., along their line of intersection. The dihedral angle ϕ_{AB} between two planes denoted A and B is the angle between their two normal unit vectors $\mathbf{n}_A$ and $\mathbf{n}_B$

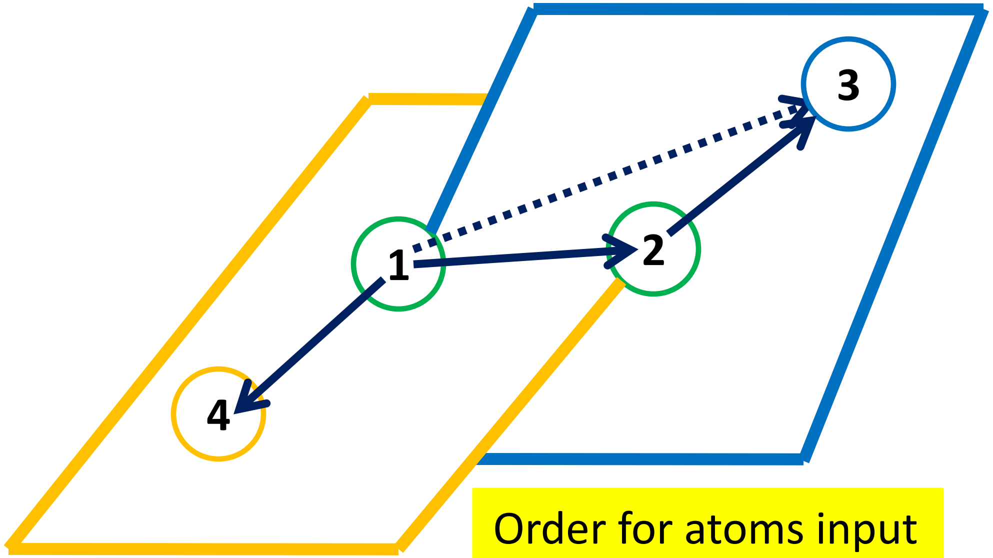
$$\cos\phi_{AB} = \mathbf{n}_A \cdot \mathbf{n}_B .$$




D
B
C
A
D
B
C
A
n
m
n
m
A

Input file for torangles

<filename>.TOR.dat



Order for atoms input

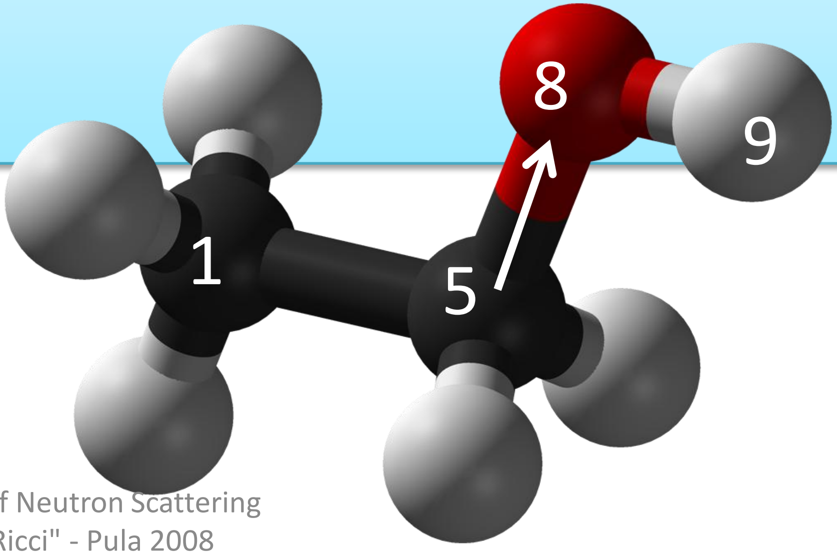
```
eth4wat6.TOR   Title of thi
fnameato       eth4wat6.ato
nsize   180    Number of co
nsumt   198    Number of co
ndist   2      Number of tr

torangles 1

atom1   CM     Atom type to define which molecule type
ltyp1   5      First atom number to define the axis
ltyp2   8      Second atom number to define the axis
ltyp3   1 1    Two atom numbers for vector from atom 1
ltyp4   9 9    Two atom numbers for vector from atom 2

torangles 2

atom1   CM     Atom type to define which molecule type
ltyp1   1      First atom number to define the axis
ltyp2   5      Second atom number to define the axis
ltyp3   2 3    Two atom numbers for vector from atom 1
ltyp4   6 7    Two atom numbers for vector from atom 2
q
```

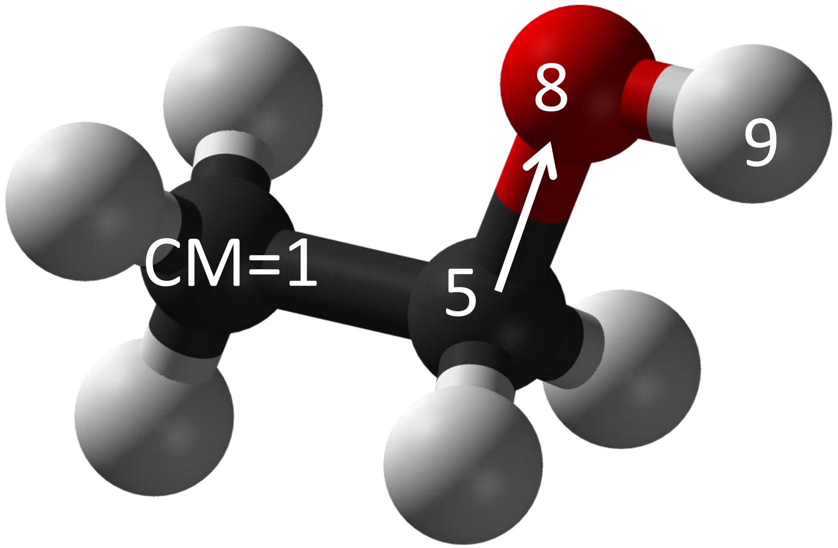
.mol file

```
4
|   |1  |2  | 3 | 4 | 5 | 6 |7  |8  |9  |10 |11 |12 |13 |14 |15 |16 |17 |18 |19
 1                  CM  *  3HM
 2                  *
 3                  CC  *  2HM
 4                  *
 5                  O   *   H
....
```

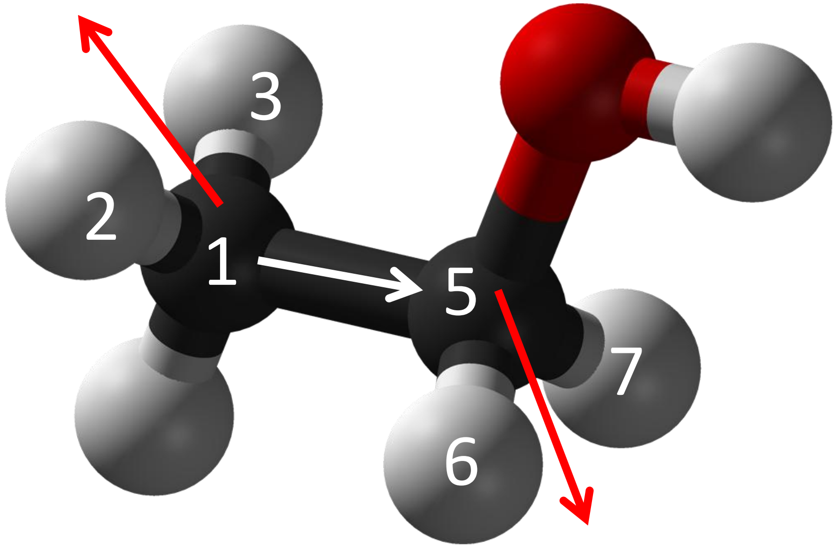
.atm file

```
4
|   |1  |2  | 3 | 4 | 5 | 6 |7  |8  |9  |10 |11 |12 |13 |14 |15 |16 |17 |18 |19
 1                  1   *  32
 2                  *
 3                  5   *  26
 4                  *
 5                  8   *   9
```





```
eth4wat6.TOR   Title of thi
fnameato       eth4wat6.ato
nsize    180   Number of co
nsumt    198   Number of co
ndist    2     Number of tr

torangles 1

atom1    CM    Atom type to define which molecule type
ltyp1    5     First atom number to define the axis
ltyp2    8     Second atom number to define the axis
ltyp3    1 1   Two atom numbers for vector from atom 1
ltyp4    9 9   Two atom numbers for vector from atom 2

torangles 2

atom1    CM    Atom type to define which molecule type
ltyp1    1     First atom number to define the axis
ltyp2    5     Second atom number to define the axis
ltyp3    2 3   Two atom numbers for vector from atom 1
ltyp4    6 7   Two atom numbers for vector from atom 2
q
```



```
eth4wat6.TOR   Title of thi
fnameato       eth4wat6.ato
nsize    180   Number of co
nsumt    198   Number of co
ndist    2     Number of tr

torangles 1

atom1    CM    Atom type to define which molecule type
ltyp1    5     First atom number to define the axis
ltyp2    8     Second atom number to define the axis
ltyp3    1 1   Two atom numbers for vector from atom 1
ltyp4    9 9   Two atom numbers for vector from atom 2

torangles 2

atom1    CM    Atom type to define which molecule type
ltyp1    1     First atom number to define the axis
ltyp2    5     Second atom number to define the axis
ltyp3    2 3   Two atom numbers for vector from atom 1
ltyp4    6 7   Two atom numbers for vector from atom 2
q
```

Basic	**What for**	**How to (theory)**	**How to (practice)**
Triangles		Analytical geometry (from the set of coordinates)	•Setup **<program>** <input filename.dat> • Input and Output files format • Commands that can be run either as one-offs or repeatedly in a script file • Plot routines
Torangles			
Clusters calculates the distribution of cluster sizes involving molecules which are at specified distances	Percolation (methane-water mixture)		

Basic	What for	How to (theory)	How to (practice)
Triangles		Analytical geometry (from the set of coordinates)	•Setup **<program>** <input filename.dat> • Input and Output files format • Commands that can be run either as one-offs or repeatedly in a script file • Plot routines
Torangles			
Clusters	Percolation (methane-water mixture)		
Chains calculates the distribution of chains among molecules and atoms which satisfy specific distance constraints, using the “shortest path” criterion to estimate the chain length between two atoms.			
Rings calculates the distribution of rings among molecules and atoms which satisfy specific distance constraints, using the “shortest path” criterion.			

Percolation (methane-water mixture)

FIG. 3. Snapshot of an experimentally constrained EPSR model of the methanol-water mixture at $x = 0.54$ showing clusters of the segregated components. Methyl groups are shown as black spheres, large white spheres high light the position of water molecules, and small gray spheres denote methanol oxygen atoms.

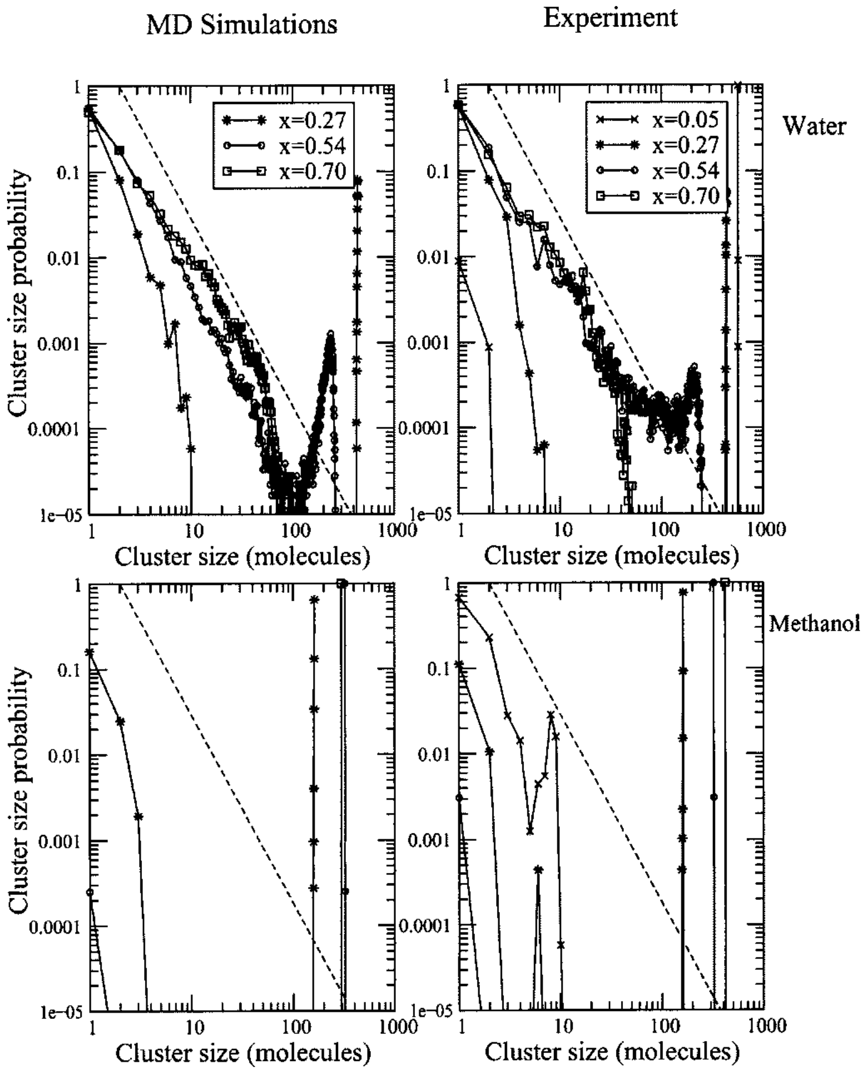


FIG. 4. Cluster size distributions for water (top) and methanol (below) clusters in methanol-water mixtures. For water molecules the hydrogen-bond definition was used to designate which molecules belong to a given water cluster, while for methanol clusters the C-C distance definition was used. On the left, from MD simulations with methanol mole fractions 0.27, 0.54, and 0.7 and on the right from neutron diffraction experiments for methanol mole fractions 0.05, 0.27, 0.54 and 0.7. The dashed lines show the predicted cluster size distribution at the percolation threshold (Ref. 36). Percolation in the simulated box occurs when clusters of a size close to the number of molecules in the simulation box form (vertical lines on the right hand side of the plot).

L.Dougan J.Chem.Phys.121, 6456 (2004)

Input file for clusters

```
mw73.CLUSTERS                    Title of this file
fnameato         mw73.ato         Name of .ato file
nsize    1000    Maximum cluster size (max 1000)
nsumt    -1      Number of configurations already accumulated
ndist    3       Number of cluster distributions

cluster 1
atom1    C       Atom type 1 to define a bond
atom2    C       Atom type 2 to define a bond
rmin     2       Minimum distance for this bond
rmax     5.5     Maximum distance for this bond

cluster 2
atom1    O       Atom type 1 to define a bond
atom2    H       Atom type 2 to define a bond
rmin     1       Minimum distance for this bond
rmax     2.5     Maximum distance for this bond

cluster 3
atom1    OW      Atom type 1 to define a bond
atom2    HW      Atom type 2 to define a bond
rmin     1       Minimum distance for this bond
rmax     2.5     Maximum distance for this bond
Q
```

Output:

mw73.CLUSTERS.n01

```
Cluster 1: fraction containing 2 or more molecules 1.00000
Cluster 2: fraction containing 2 or more molecules 0.79762
Cluster 3: fraction containing 2 or more molecules 0.72222
```

It's also the output…

Compared to **clusters**, the **chains** program uses a **more advanced criterion for deciding whether two molecules are bonded or not**.

The program calculates 2 distributions for each chain definition.

- The first is the distribution of bond numbers, i.e. how many bonds are there per valid molecule.

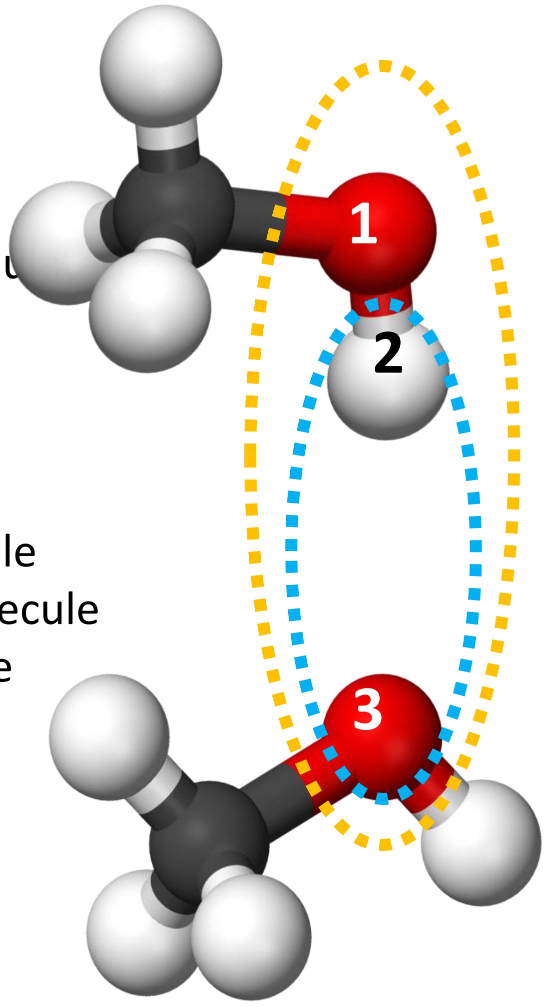
- The second is the chain length distribution.

The chain length is calculated using the “shortest path” criterion, which basically sorts through all the possible linked paths between two molecules, and counts only the shortest path, i.e. the one with the least number of linkages between those two molecules.

- Each **chain** must begin and end on a molecule with only one link to another molecule.

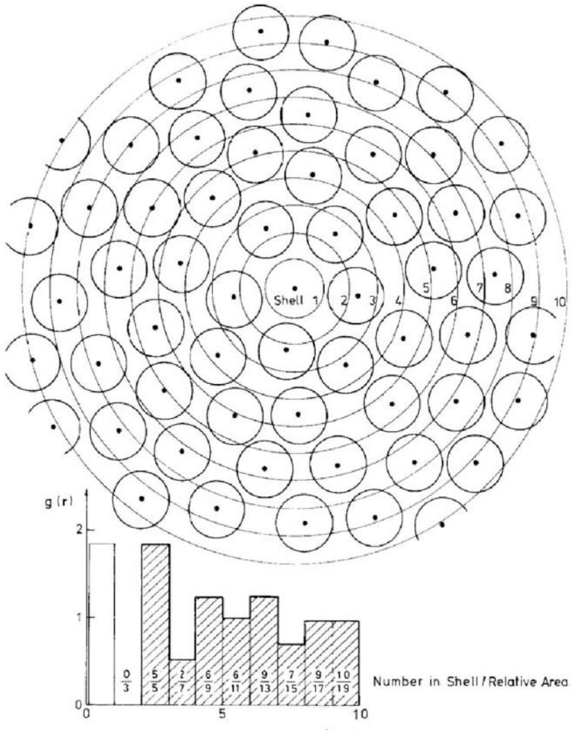
- The only difference between the two routines is that a **ring** can only begin and end on a molecule with two or more linkages.

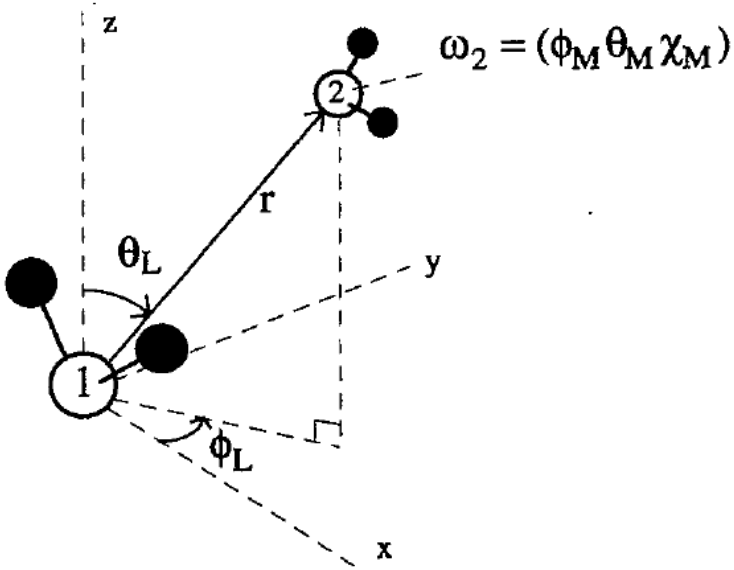
Input file for CHAINS and RINGS



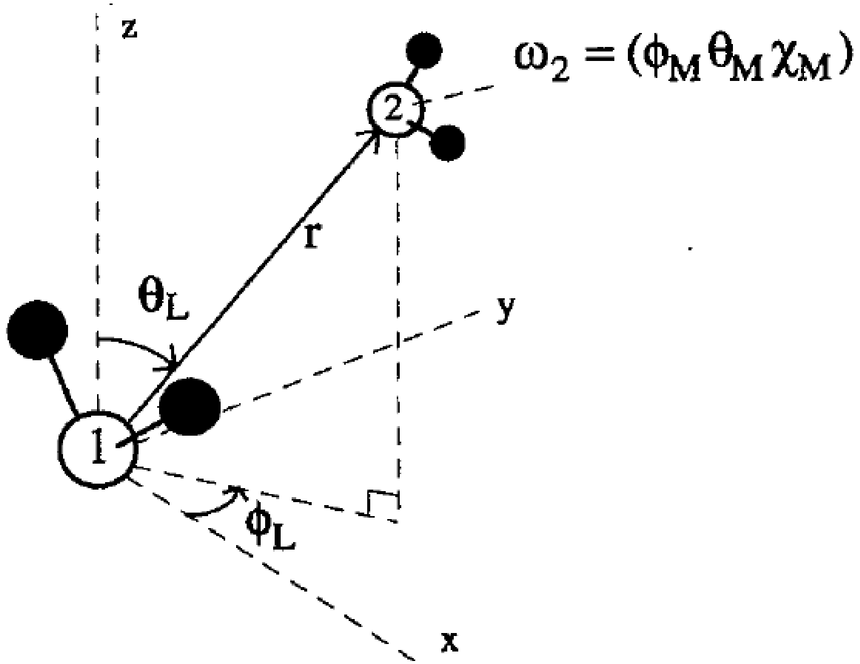
```
methanol.CHAINS                  Title of this file
fnameato             methanol1.ato       Name of .ato file
nsize     200        Maximum chain length (max 200)
nsumt     -1         Number of configurations already accumu
ndist     1          Number of chain length distributions

chain     1

atom1     O          Atom type 1 for first atom in first molecule
atom2     H          Atom type 2 for second atom in first molecule
atom3     O          Atom type 3 for atom in second molecule
rmin1     1          Minimum distance for atom1-atom3
rmax1     3.4        Maximum distance for atom1-atom3
rmin2     1          Minimum distance for atom2-atom3
rmax2     2.5        Maximum distance for atom2-atom3
q

1 0.17900E+01 0.63511E+00 0.58000E+01 0.48229E+01
```

Advanced	What for	How to (theory and practice)
Sharm and SDF calculates the spherical harmonic coefficients for the Spatial Density Function (SDF) and the Orientational Correlation Function (OCF)	•The peculiar case of Hydrogen Bond in H_2O and H_2S •NaOH in Water	1. Minimum Noise approach to a “heavily undetermined" problem 2. Spherical Harmonics representation of g(**r**)





Where I explain why explicit calculation is not so convenient…



"Once you get away from the cosy world of pair distribution functions, you run into two problems"

- **How to store a function of 3 to 6 variables**

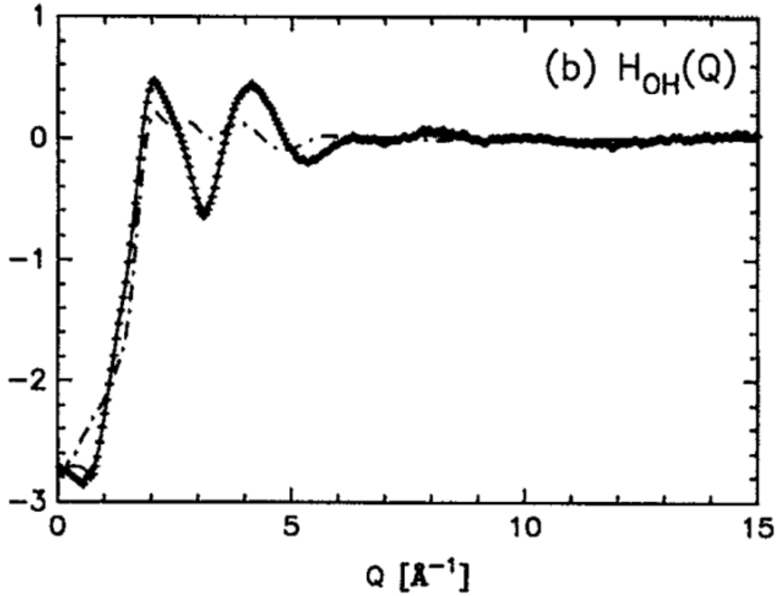
For example, the orientational correlations for two arbitrary shaped molecules with little symmetry:

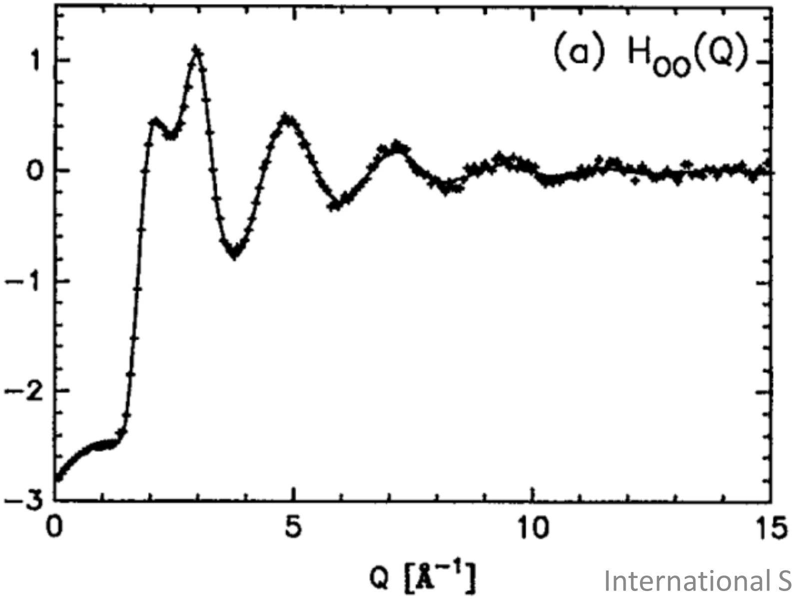
  - Digitize a radial grid into 100 steps
  - Digitize each angle into 9º steps: 20θL, 40ϕL, 20θM, 40ϕM, 40χM

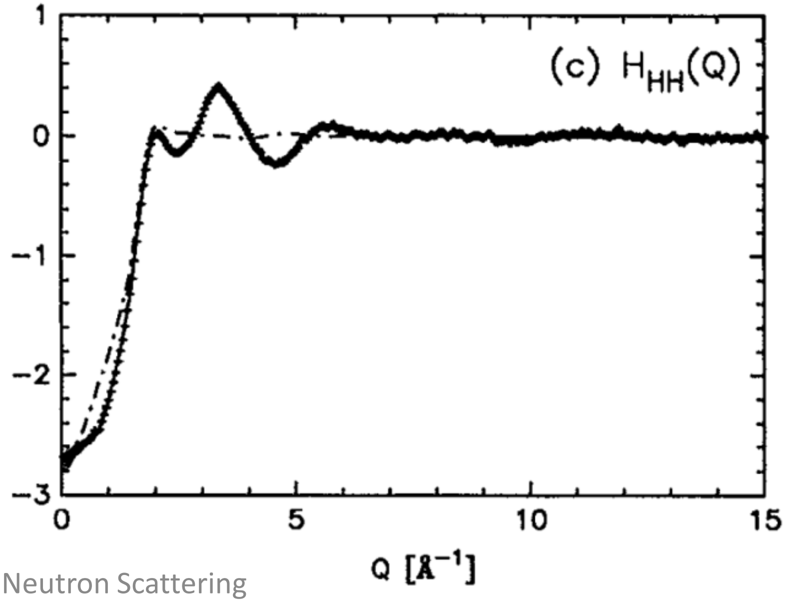
Total number of pixels = 2560000000 = 2.59×10^9

- **How to visualize the output (given that we can understand maximum 3 dimensions)**

Measured partial structure factors for water as obtained in a recent SANDALS experiment. The crosses show the actual data, the solid lines show the fit to these data using the full spherical harmonic expansion and the dashed-dotted lines show the result of assuming the water molecules have isotropic relative orientations.







Measured partial structure factors for hydrogen sulfide (symbols) and their minimum noise fit

“While fully admitting that there is no direct route to the complete orientational correlation function in a molecular liquid, it is nonetheless a very reasonable question to ask **what would be the least amount of structure in that correlation function that could be sustained**, given that there are some measured partial structure factor data available, and given that the liquid is made up of molecules of known geometry.”

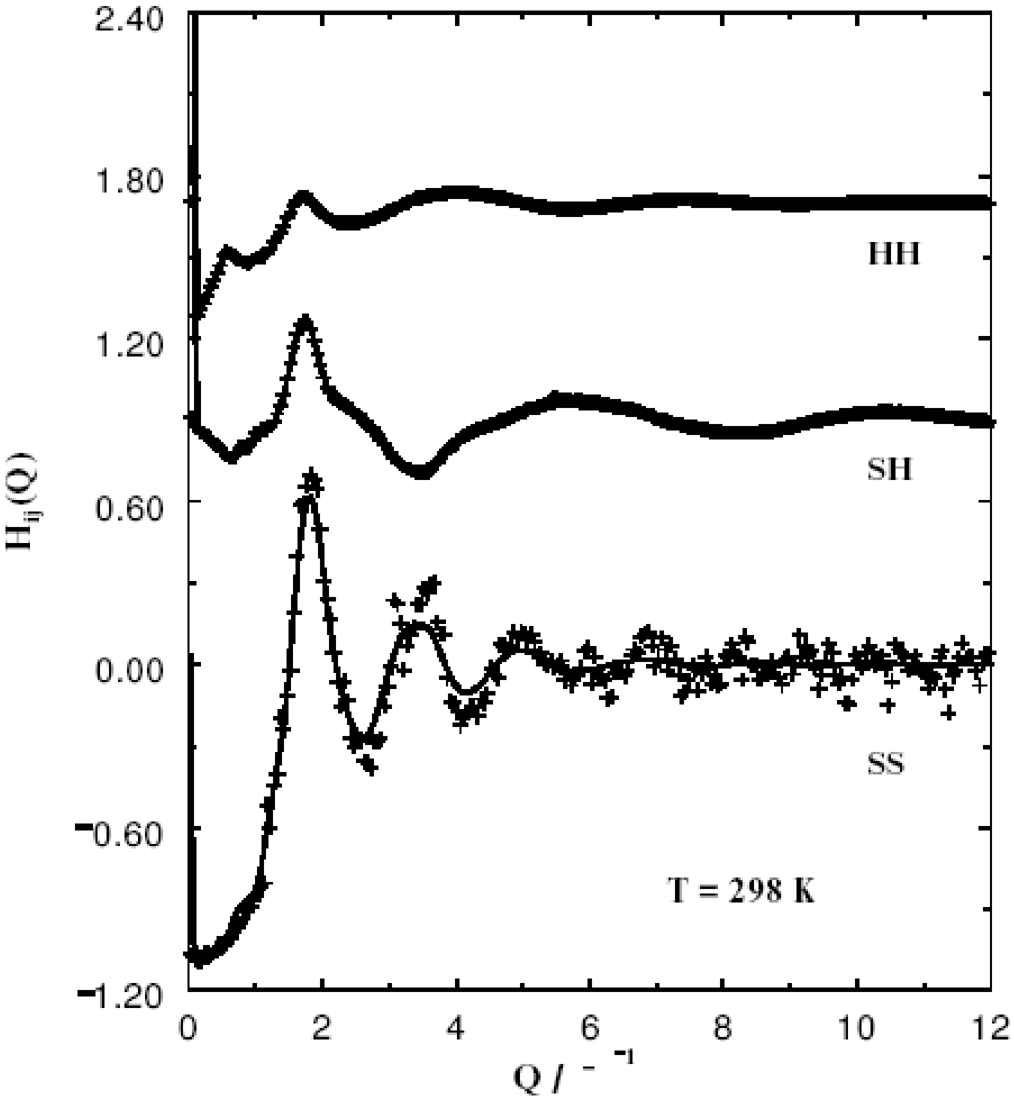


Figure 2. Partial structure factors measured at $T = 298$ K (symbols) and their minimum noise fit (solid line); sulphur–hydrogen and hydrogen–hydrogen factors have been shifted by an arbitrary quantity.

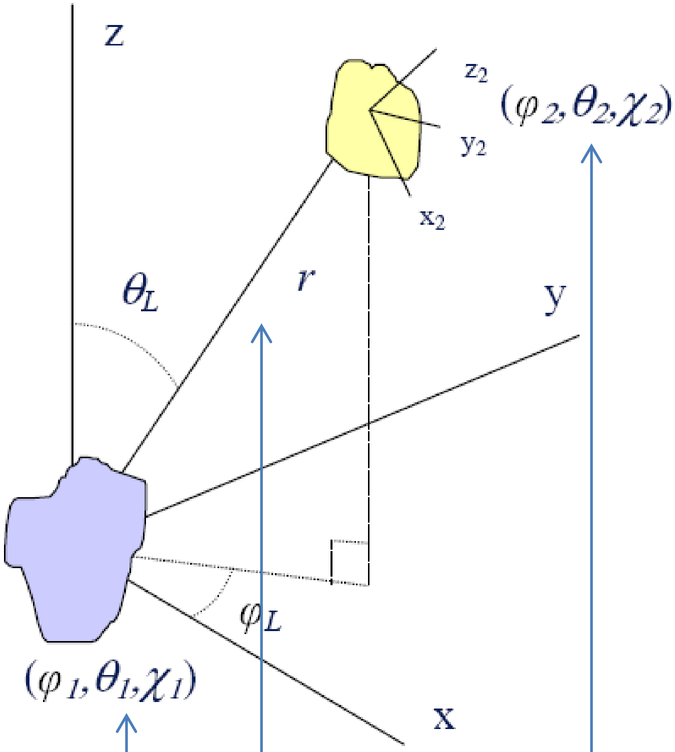
The **site-site partial structure factors can be expanded as a series of spherical harmonic functions**

- Generalized rotation matrix

$$D^l_{mn}(\omega) = e^{-im\phi} d^l_{mn}(\theta) e^{-in\chi}$$

- Clebsch-Gordan coefficients

$$|l_1 - l_2| \le l \le l_1 + l_2 \text{ and } m = m_1 + m_2$$



$$h(\mathbf{r},\omega_1,\omega_2) = \sum_{l_1 l_2 l} \sum_{m_1 m_2 m} \sum_{n_1 n_2} h(l_1 l_2 l; n_1 n_2; r)$$

$$\times C(l_1 l_2 l; m_1 m_2 m) \boxed{D^{l_1}_{m_1 n_1}(\omega_1)^*}$$

$$\times \boxed{D^{l_2}_{m_2 n_2}(\omega_2)^*} \boxed{D^{l}_{m0}(\omega)},$$

$$H_{\alpha\beta}(Q)=4\pi\rho\int_0^\infty r^2[g_{\alpha\beta}(r)-1]\,\frac{\sin Qr}{Qr}\,dr.$$

$$h(\mathbf{r},\omega_1,\omega_2)\ [=g(\mathbf{r},\omega_1,\omega_2)-1]$$

Both the Q side and the r side can be expanded…

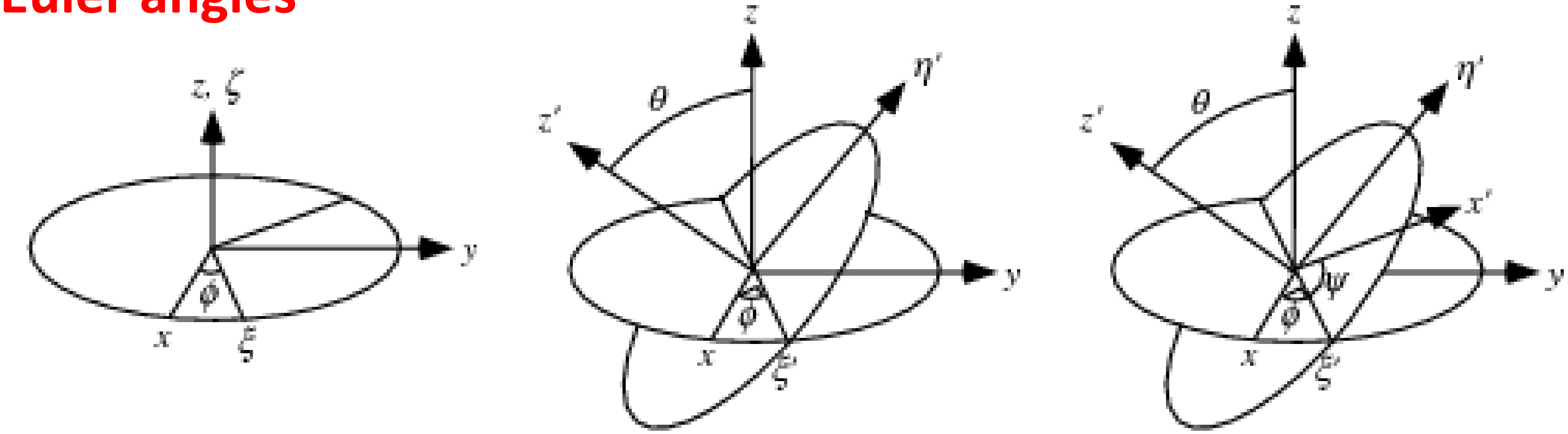
$h(\mathbf{r},\omega_1,\omega_2)$ See previous slide…

$$H(Q)=\sum_{l_1l_2l}\sum_{n_1n_2}f(l_1l_2l)C(l_1l_2l;000)H(l_1l_2l;n_1n_2;Q)$$
$$\times[F_{l_1n_1}(Q)\times F_{l_2n_2}(Q)],$$

The coefficients for each expansion are related by a fourier bessel transform

$$H(l_1l_2l;n_1n_2;Q)=4\pi\rho\int_0^\infty r^2h(l_1l_2l;n_1n_2;r)j_l(Qr)dr$$

Euler angles



To perform a transformation from the fixed starting coordinate reference system to a relative reference frame XYZ→xyz, the convention adopted was
(i) to rotate positively in the advancing direction of a right hand screw, through an angle ϕ (0°≤ϕ≤360°) about the Z axis, XYZ→X'Y'Z',

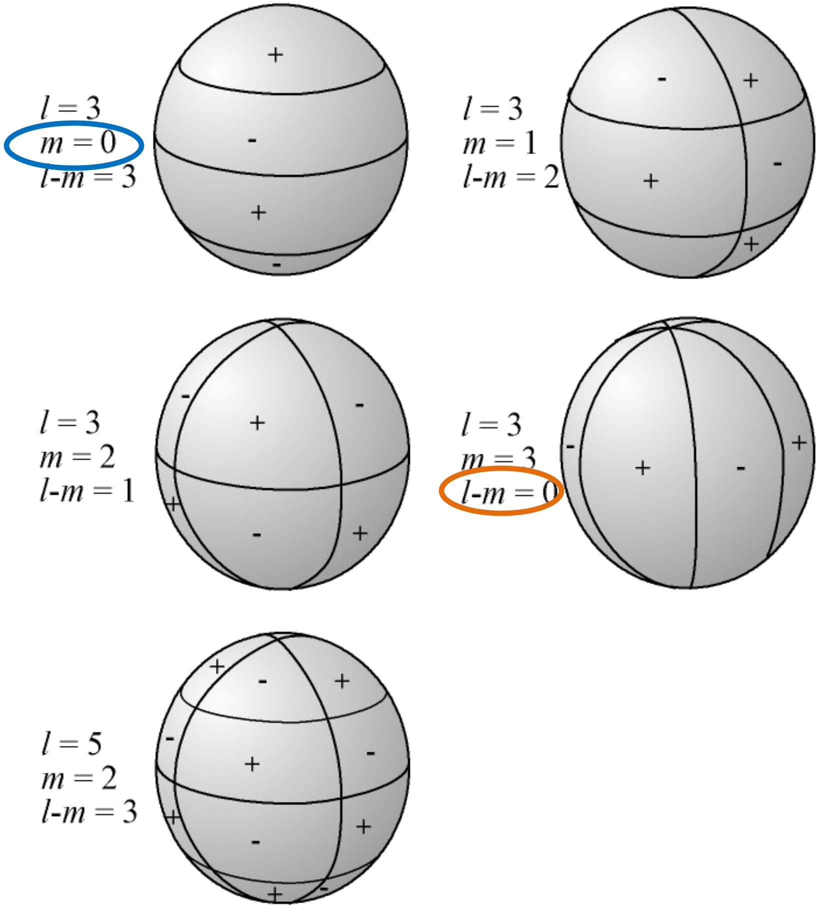
(ii) rotate by θ (0°≤θ≤180°) about Y‘, X'Y'Z'→X”Y”Z”, and finally

(iii) rotate by χ (0°≤χ≤180°) about Z” to bring X”Y”Z”→xyz

Ok but, how do they look like?

$$Y_\ell^m(\theta,\varphi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\varphi}$$

The spherical harmonics are **easily** visualized by counting the number of zero crossings they possess in both the latitudinal and longitudinal directions. For the latitudinal direction, the associated Legendre functions possess *l* − | *m* | zeros, whereas for the longitudinal direction, the trigonomentric sin and cos functions possess 2 | *m* | zeros. When the spherical harmonic order *m* is zero, the spherical harmonic functions do not depend upon longitude, and are referred to as zonal. When *l* = | *m* | , there are no zero crossings in latitude, and the functions are referred to as sectoral. For the other cases, the functions checker the sphere, and they are referred to as tesseral.



Schematic representation of Y_{lm} on the unit sphere. Y_{lm} is equal to 0 along m great circles passing through the poles, and along l-m circles of equal latitude. The function changes sign each time it crosses one of these lines.

Input file for SHARM

```
h2o298tot.SHARM                    Title of this file
fnameato             h2o298tot_s.ato     Name of .ato file
nr          130                    Number of radius values (max 200)
rmax        13                     Maximum radius for spherical harmonic coefficients
nsumt       1                      Number of configurations already accumulated

ncoeffs     158                    Number of coefficients (program calculates this)
l1values    0 1 2 3 4              L1 values (separated by spaces)
l2values    0 1 2 3 4              L2 values (separated by spaces)
lvalues     0 1 2 3 4              L values (separated by spaces)

n1step      2                      Step in N1 values
n2step      2                      Step in N2 values

atom-c      OW                     Central molecule - list of centre atom types
axisc1      z 2 3                  First axis definition for central molecule
axisc2      y 2                    Second axis definition for central molecule

atom-s      OW                     Second molecule - list of centre atom types
axiss1      z 2 3                  First axis definition for second molecule
axiss2      y 2                    Second axis definition for second molecule
q
```

Input file for SDF

```
sio2_095.SDF               Title of this file
fnameato    sio2_095.ato               Name of .ato file
nr          130               Number of radius values (max 200)
rmax        13               Maximum radius for spherical harmonic coefficients
nsumt       1               Number of configurations already accumulated
ncoeffs     16               Number of coefficients (program calculates this)
l1values    0 1 2 3 4 5 6               L1 values (separated by spaces)
l2values    0               L2 values (separated by spaces)
lvalues     0 1 2 3 4 5 6               L values (separated by spaces)
n1step      2               Step in N1 values
n2step      0               Step in N2 values
atom-c      Si O O          List of centre atom types. First will be origin.
pairdist-c  1.6 1.6 2.6     List of pair distances for centre molecule.
fracdist-c  0.2             Acceptance half-width (fraction of pair distance).
axisc1      z 2 3           First axis definition for centre molecule.
axisc2      y 2             Second axis definition for centre molecule.
atom-s      O               List of second atom types. First will be origin.
pairdist-s  0               List of pair distances for second molecule.
fracdist-s  0.2             Acceptance half-width (fraction of pair distance).
axiss1      z               First axis definition for second molecule.
axiss2      y               Second axis definition for second molecule.
q
```

The power of the method

The power of the method arises from the fact that awkward integrals over angular coordinates are replaced by simple sums over the coefficients

The spherical harmonic representation is an extremely compact method of storing many-body correlation functions.

The added bonus is that having calculated the coefficients you can go back and interrogate the distribution in various ways without having to recalculate the atom positions all over again.

Sharm and SDF **Calculates the spherical harmonic coefficients** for the Spatial Density Function (SDF) and the Orientational Correlation Function (OCF)
PLOT2D and **PLOT3D** This is where I really to integrate over a certain variable or over a different one

Input file for PLOT3D

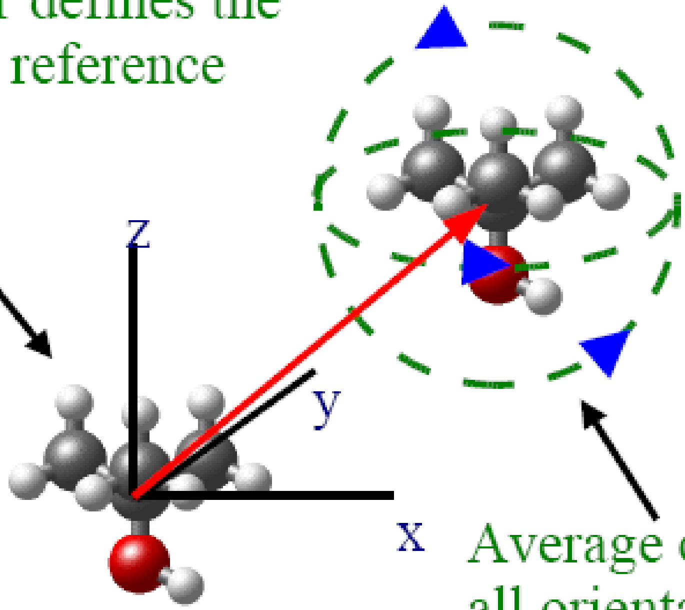
Basically once the coefficients have been calculated you can choose how to sum the up (this step is equivalent to an integration in one of the variables) and this is done directly in the plot routine

```
sio2_095.SDF.h01
16                 no. of coefficients - determined from coefficients file
1                 = 0 for identical molecules, else 1 if different
1                 0 sets first coefficient to zero - normally 1
4                 number of smoothings on coefficients
6                 maximum radius of plotting box
1 1                 no. of plots along x- and y-axis [set at 1 1]
1.0                 aspect ratio of plot [1.0]
1 6                 minimum and maximum radius of plot
0.2                 fractional isosurface level (-ve for absolute)
1 0                 use l1 and l2 (1 or 0)
1 0                 use n1 and n2 (1 or 0)
0                 use m (1 or 0)
1                 vary (thetal, phil) (1), (thetam, phim) (2), (thetam, chim) (3)
0 0 0
```

…etc

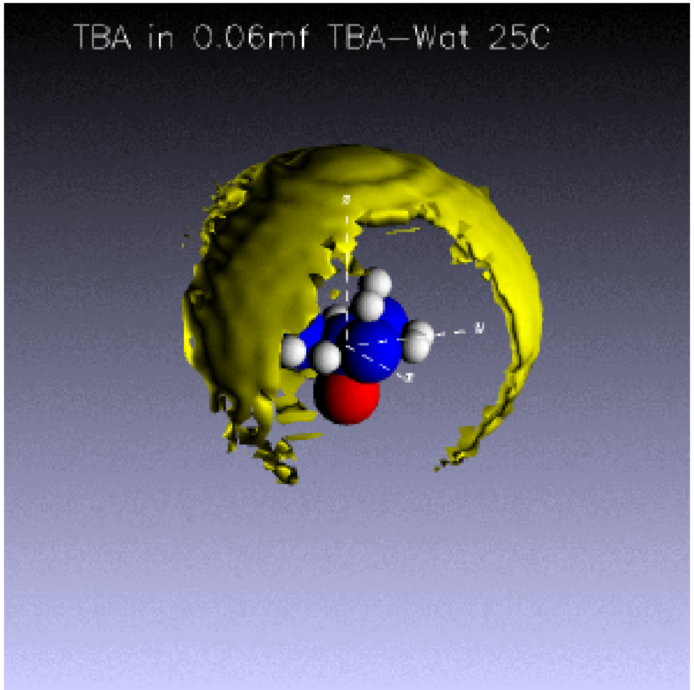
Spatial Density/Distribution Functions (SDF's)

The spatial density function, $g(\mathbf{r},\Omega)$, represents the probability of finding a neighbouring molecule as a function of radial distance $\mathbf{r}$ and orientation Ω, about a central molecule defining the coordinate reference frame.



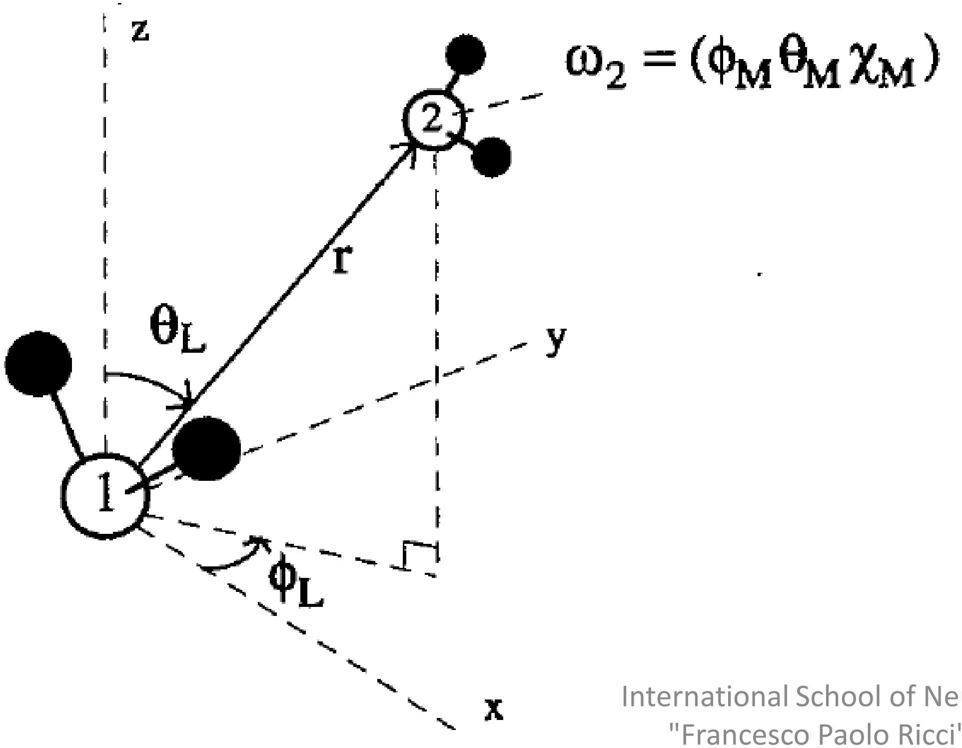
Molecule 1 defines the coordinate reference frame

Average over all orientations of molecule 2



```
1 0              use l1 and l2 (1 or 0)
1 0              use n1 and n2 (1 or 0)
0               use m (1 or 0)
1               vary (thetal, phil) (1), (thetam, phim) (2), (thetam, chim) (3)
0 0 0
```

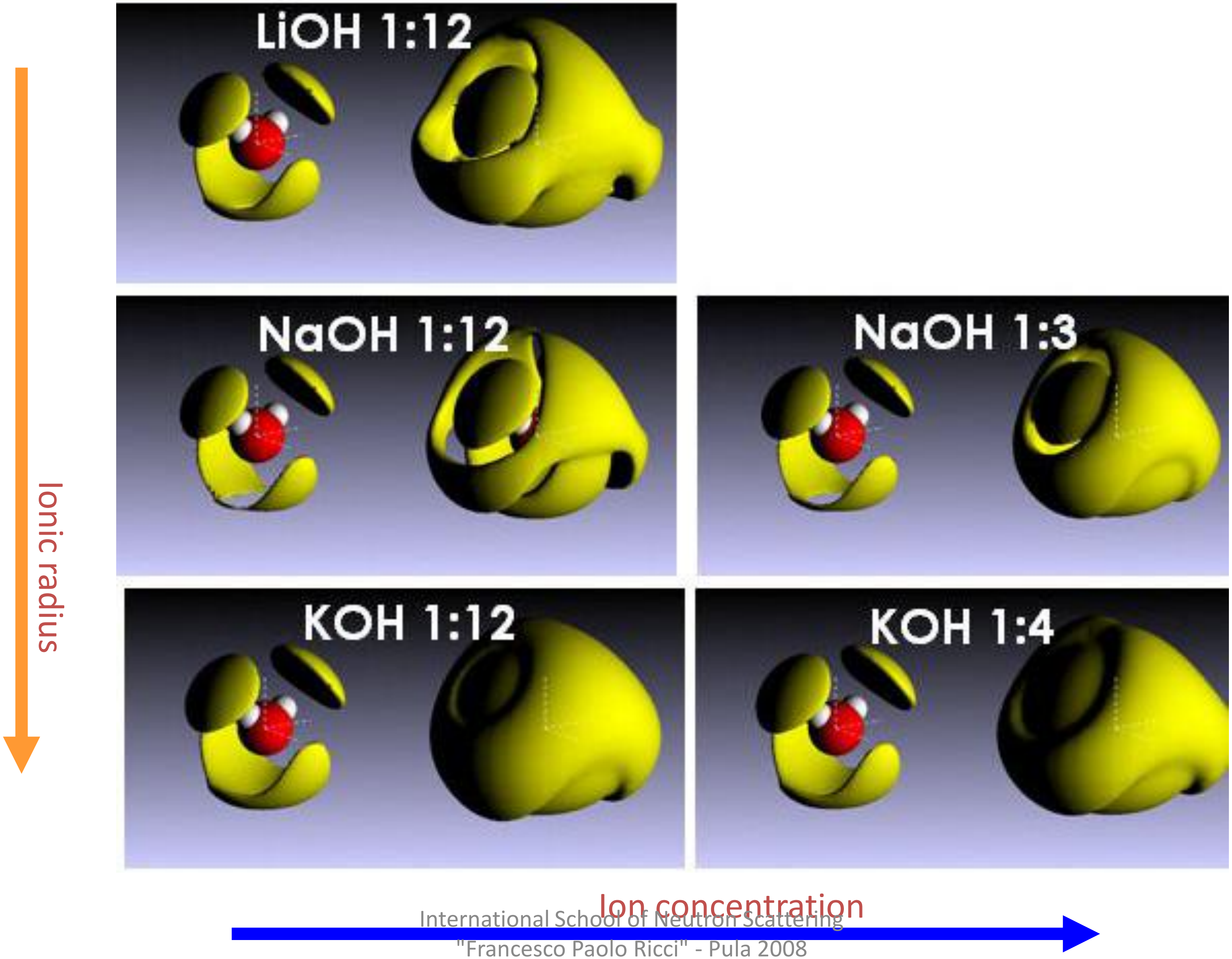
$$D^{l}_{mn}(\omega)=e^{-im\phi}d^{l}_{mn}(\theta)e^{-in\chi}$$



Euler angle	“Quantum” no.
f	m
q	lmn
c	n

Relative position		Orientation of molecule 2	
l1 (l)	1	l2	0
n1 (n)	1	n2	0
		m2	0

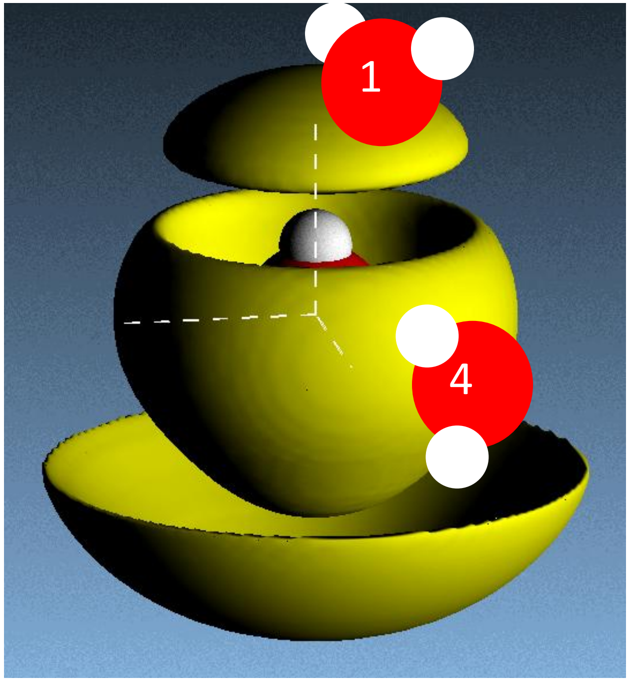
Water –water correlations

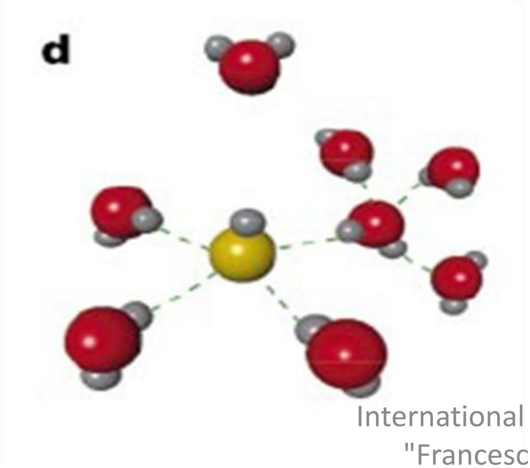


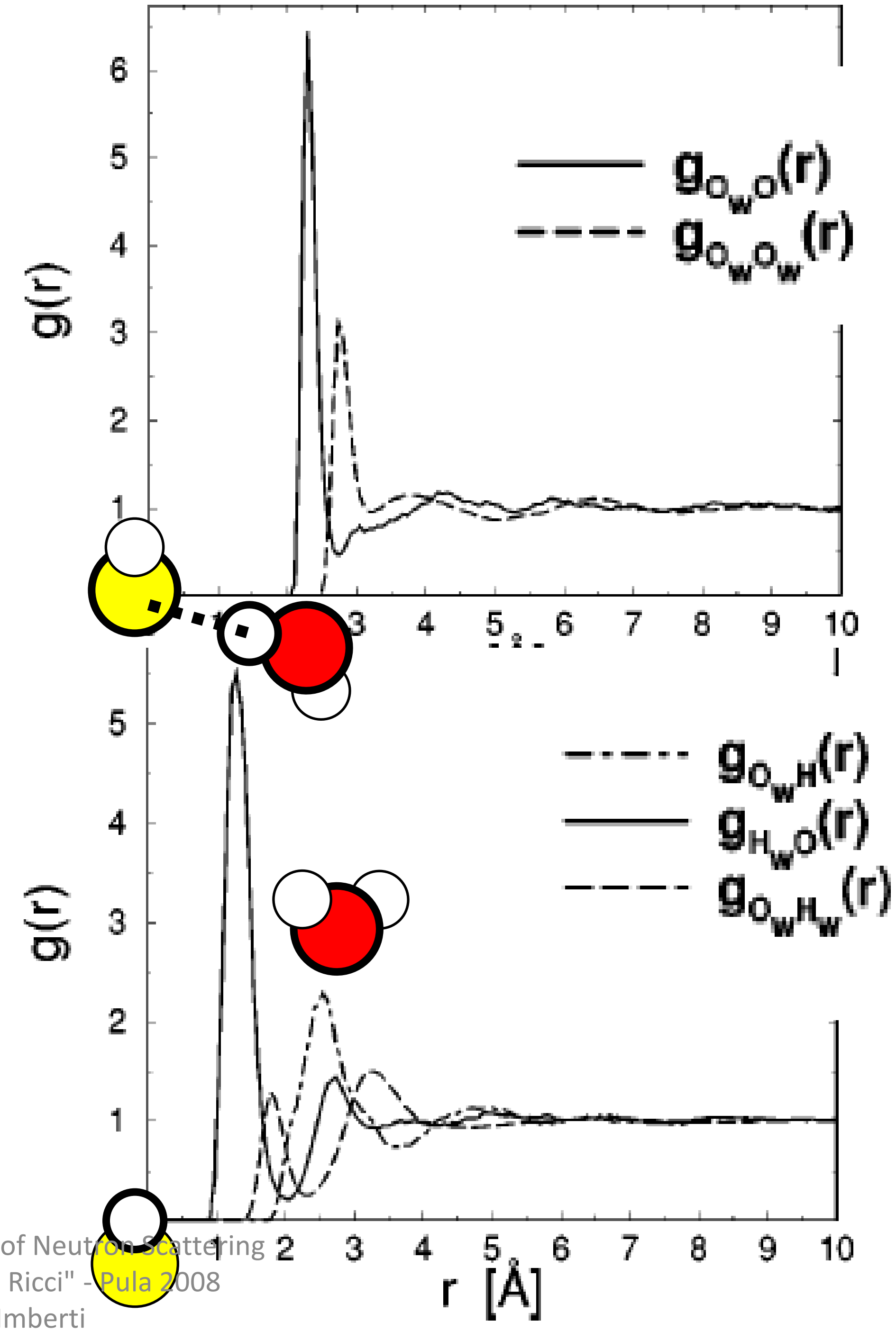
Ionic radius

Ion concentration

Hydroxyl ion solvation shell



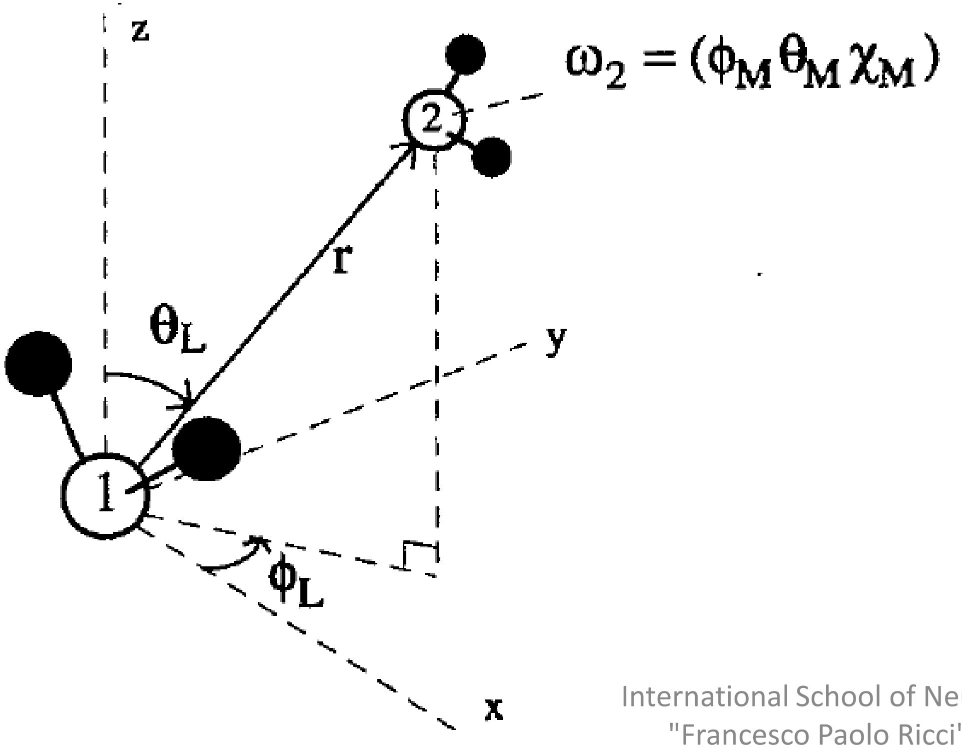




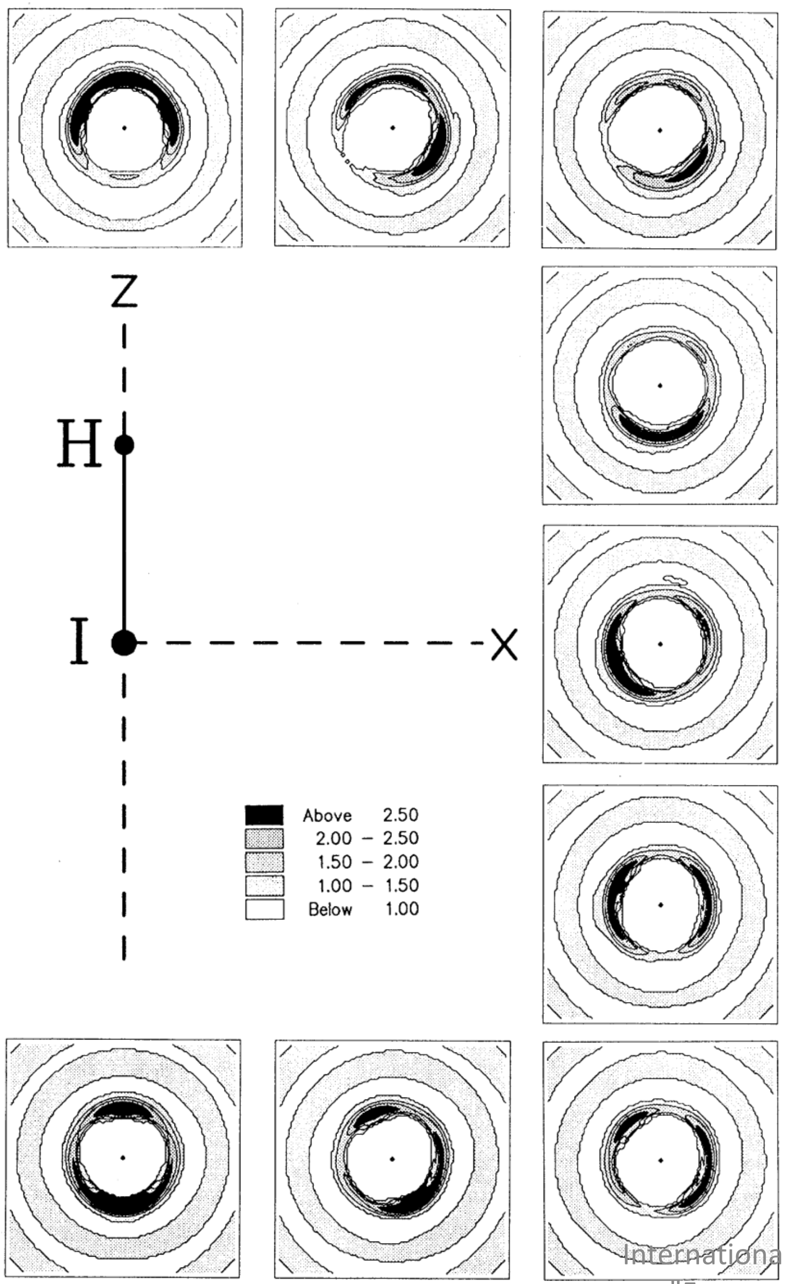
```
1 0                  use l1 and l2 (1 or 0)
1 0                  use n1 and n2 (1 or 0)
0                  use m (1 or 0)
1                  vary (thetal, phil) (1), (thetam, phim) (2), (thetam, chim) (3)
0 0 0
```

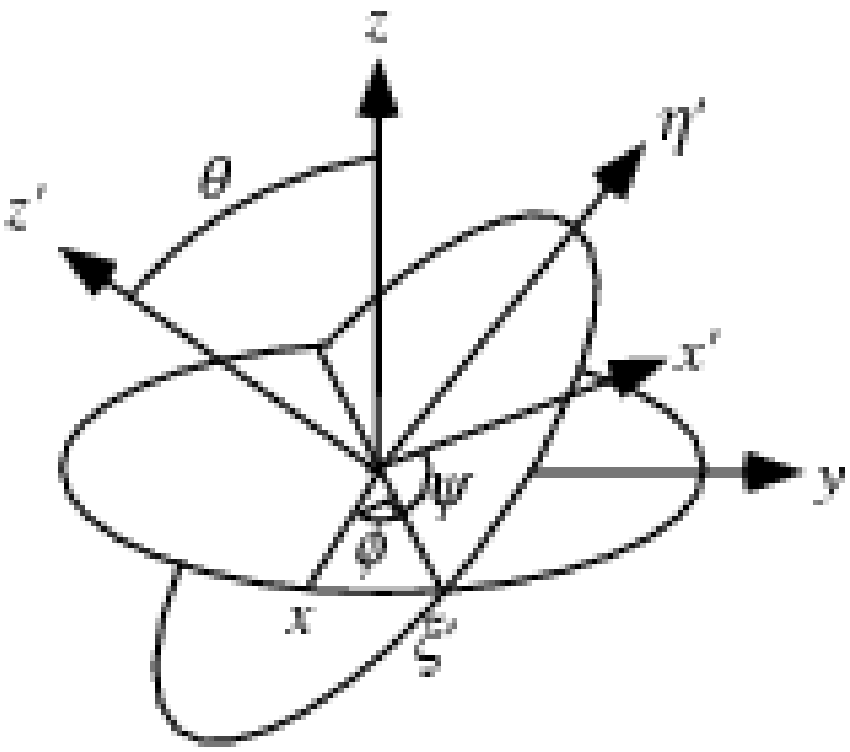
$$D^{l}_{mn}(\omega) = e^{-im\phi} d^{l}_{mn}(\theta) e^{-in\chi}$$

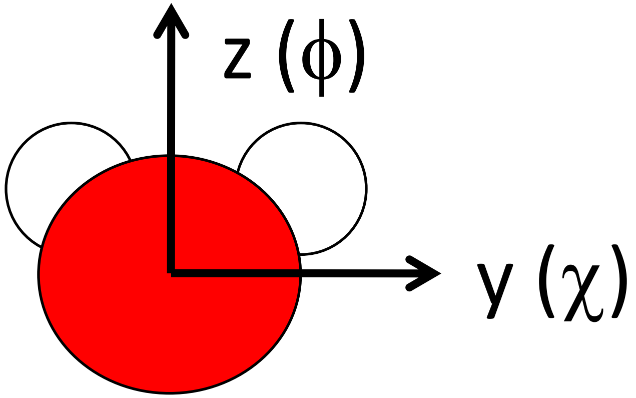
Euler angle	“Quantum” no.
f	m
q	lmn
c	n



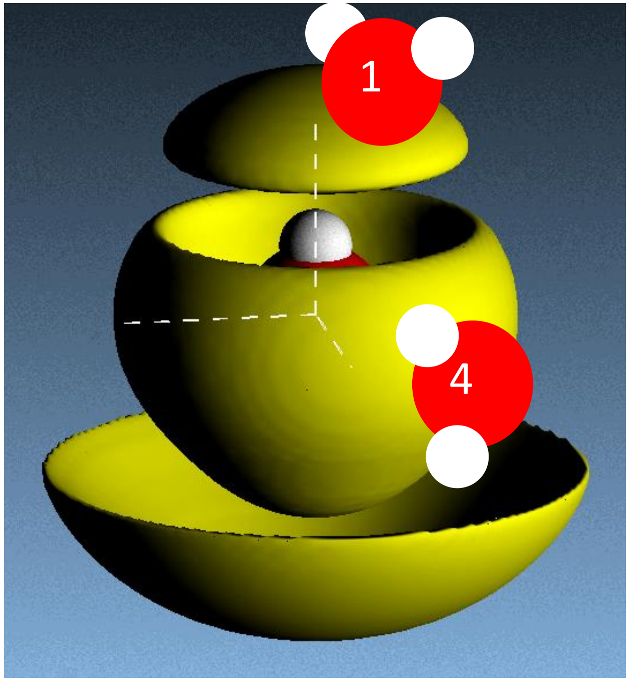
Relative position		Orientation of molecule 2	
l1 (l)	1	l2	1
n1 (n)	1	n2	1
		m2	1

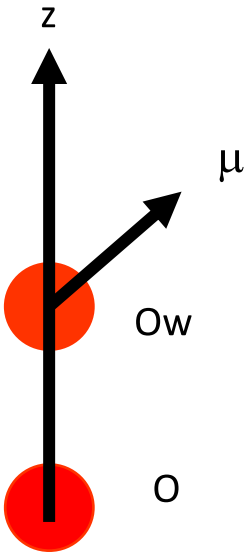

Z
H
I
X
■ Above 2.50
▨ 2.00 – 2.50
▨ 1.50 – 2.00
▨ 1.00 – 1.50
☐ Below 1.00

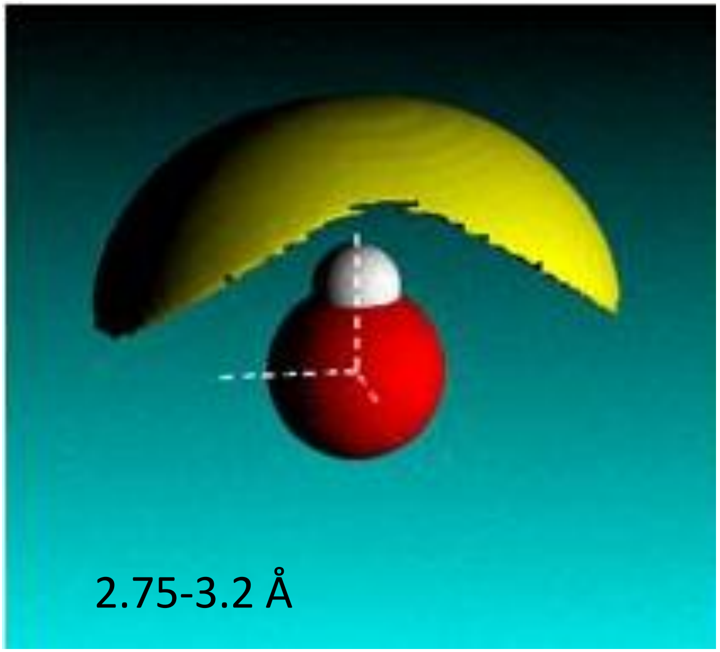

z
η'
θ
z'
x'
y
ψ
φ
x
ξ


z (ϕ)
y (χ)

```
1 1                     #11 if zero use only l1=0 and/or l2=0
1 1                     #12 if zero use only n1=0 and/or n2=0
1                       #13 if zero use only m2=0
3                       #14 vary thetal and phil(1) thetam and phim(2), or thetam and chim(3) for second molecule
```







The most exciting phrase to hear in science, the one that heralds new discoveries, is not “Eureka” (I’ve found it!) but “That’s funny…”

(Isaac Asimov)

Have fun!