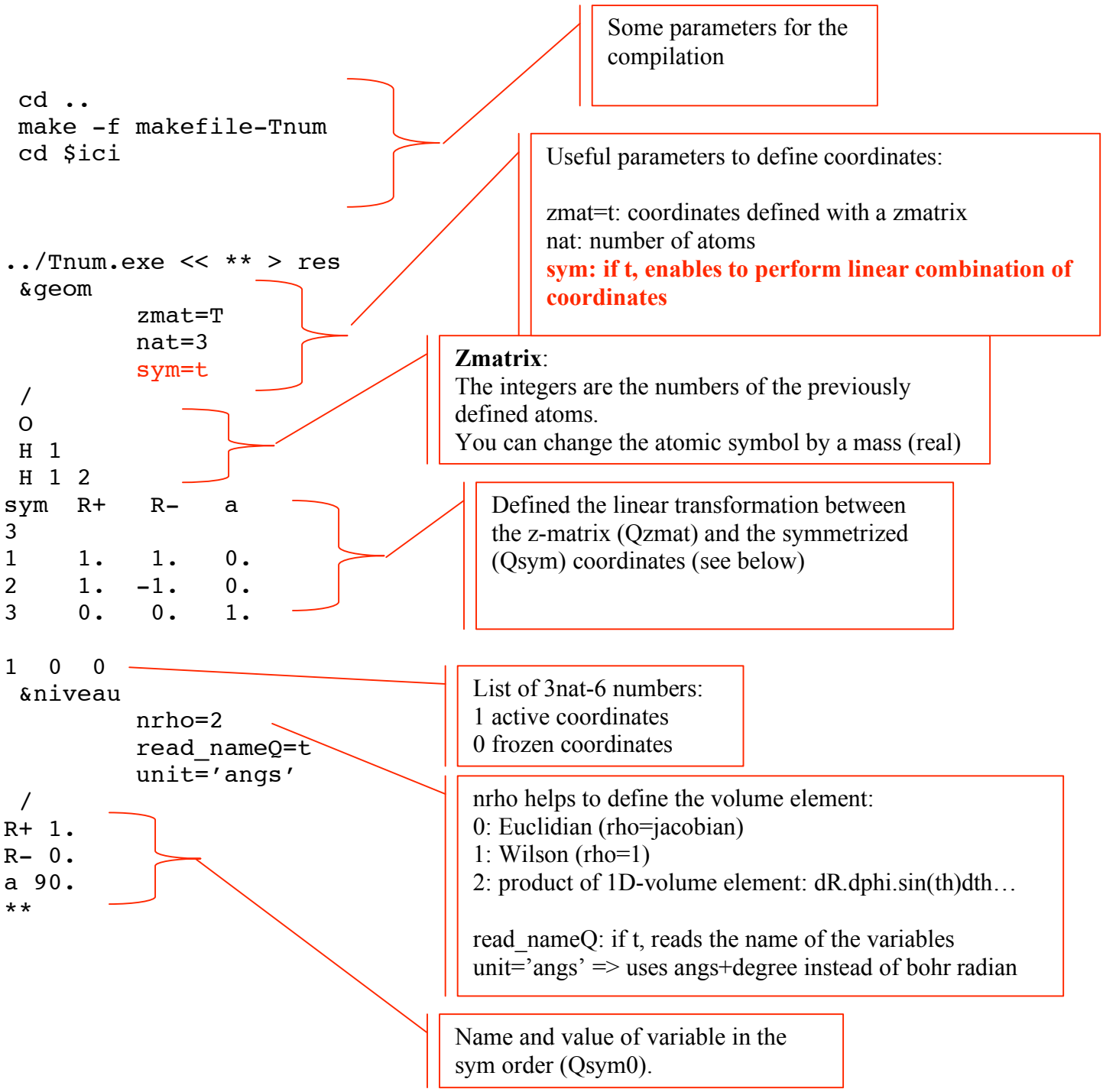
cd ..
make -f makefile-Tnum
cd $ici
../Tnum.exe << ** > res
&geom
zmat=T
nat=3
sym=t
/
O
H 1
H 1 2
sym R+ R- a
3
1 1. 1. 0.
2 1. -1. 0.
3 0. 0. 1.
1 0 0
&niveau
nrho=2
read_nameQ=t
unit='angs'
/
R+ 1.
R- 0.
a 90.
**
Some parameters for the compilation
Useful parameters to define coordinates:
zmat=t: coordinates defined with a zmatrix
nat: number of atoms
sym: if t, enables to perform linear combination of coordinates
Zmatrix:
The integers are the numbers of the previously defined atoms.
You can change the atomic symbol by a mass (real)
Defined the linear transformation between the z-matrix (Qzmat) and the symmetrized (Qsym) coordinates (see below)
List of 3nat-6 numbers:
1 active coordinates
0 frozen coordinates
nrho helps to define the volume element:
0: Euclidian (rho=jacobian)
1: Wilson (rho=1)
2: product of 1D-volume element: dR.dphi.sin(th)dth…
read_nameQ: if t, reads the name of the variables
unit='angs' => uses angs+degree instead of bohr radian
Name and value of variable in the sym order (Qsym0).

For the symmetrization, we need to set up the linear relation between the z-matrix coordinates and the symmetrized ones:

$$Qzmat(i) = \sum_k Mat(i,k) * Qsym(k)$$

Just the matrix Mat(i,k) is needed (3N-6*3N-6). It is given in the following way:

After the last atom of the z-matrix :
A comment line (not read) used to remenber the order of the symmetrized coordinates (here : R+ R- a)

sym R+ R- a

Then, an integer, n (usually the 3N-6). If n is smaller than 3N-6, the matrix will be read in several block of n columns. Here n=3

3

Then, the matrix itself. The symmetrized coordinates are in the columns and the z-matrix ones in the lines. In the first column, integers to count the lines.
For the water :

1 1. 1. 0.
2 1. -1. 0.
3 0. 0. 1.

Therefore:
Qzmat(1) = ROH1 = 1. Qsym(1) +1. Qsym(2)
Qzmat(2) = ROH2 = 1. Qsym(1) -1. Qsym(2)
Qzmat(3) = aHOH = Qsym(3)

With Qsym(1) = R+ (symmetric stretch)
Qsym(2) = R- (antisymmetric stretch)
Qsym(3) = a (bending HOH)

Be carreful: You can mix only the coordinates with the same “type” (distance, valence angle, dihedral angles). For example, you cannot mix an angle and a distance.