

```
cd ..
make -f makefile-Tnum
cd $ici
```

Some parameters for the compilation

```
../Tnum.exe << ** > res
&geom
```

```
zmat=T
nat=10
sym=f
```

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 (see dat_HCN).

```
/
H
C 1
C 2 1
C 2 1 3
H 3 2 4
H 3 2 5
H 3 2 5
H 4 2 3
H 4 2 8
H 4 2 8
```

Zmatrix:

The integers are the numbers of the previously defined atoms.

You can change the atomic symbol by a mass (real)

List of 3nat-6 numbers:
1 active coordinates
0 frozen coordinates

```
0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0
&niveau
```

```
nrho=2
read_nameQ=t
```

nrho helps to define the volume element:

0: Euclidian (rho=jacobian)
1: Wilson (rho=1)
2: product of 1D-volume element: $dR.d\phi_i.\sin(\theta)d\theta...$

read_nameQ: if t, reads the name of the variables

```
/
rH 2.06280
rCC 2.72444
aCCH 2.03908
rCC 2.72444
aCCH 2.03908
dih 3.14159
rCH21 2.09066
aCH21 1.90364
dCH21 0.00000
rCH22 2.09066
aCH22 1.90364
dCH22 2.09439510258113692
rCH23 2.09066
aCH23 1.90364
dCH23 -2.09439510258113692
rCH31 2.09066
aCH31 1.90364
dCH31 0.00000
rCH32 2.09066
aCH32 1.90364
dCH32 2.09439510258113692
```

Name and value of variable in the zmatrix order.

rCH33 2.09066
aCH33 1.90364
dCH33 -2.09439510258113692
**