```
#
# You should get the result of the Eh_exact (column 4 of table II).
# Lauvergnat et al, JCP, v114 (2001) p6592
#

 SYSTEM=sub_system_cos_hcn.f

ici=`pwd`
DIR_vib=$ici/..
DIR_pot=$DIR_vib/sub_pot

 cp $SYSTEM $DIR_pot/sub_system.f

cd $DIR_vib
 make
cd $ici

 x1=0.538516066
 x2=0.461483933


nice $DIR_vib/vib << ** >res
 &system /
 &constantes /
 &variables
          zmat=T
          nat=4
          sym=T
          nrho=2
          Qeq_sym=t
 /
C
0.0      1
N      2  1
H      2 -1 3
sym  cos(a)       R      r     x     pi    dh
6
1       0.         0.   $x1     1.    0.    0.
2       0.         0.   $x2    -1.    0.    0.
3       0.         0.   0.      0.    1.    0.
4       0.         1.   0.      0.    0.    0.
5       1.         0.   0.      0.    0.    0.
6       0.         0.   0.      0.    0.    1.

 1 21   21     0 0 0
 &minimum pot0=-0.499465823200 HarD=t /
.999d0
3.187
2.179
0.
3.14159265358979323846264338327 9d0
0.0
```

Some parameters for the compilation

Parameters for the Jacobi coordinates (Tnum)

Parameters of Tnum

Reference energy + parameter for the kind of potential,
HarD =t => the PES is split in V0+(V1)+V2

V2 : quadratic contribution

Reference geometry

```
   "nD"    0    0   F    0     0. 1.
 &basis_nD iQact(1)=1 name="Pl0" nb=51 nq=80 cte(2,1)=1. /
 &inactives
           max_excit=4
           tab_nq(1)=8,8
           tab_nb(1)=5,5
           sort=f
           max_ene_h=60000.d0 n_h=15  num=f,step=0.00001
/
 &actives test=f max_ene=20000.d0 lect=f comput_S=t
          non_adia=t restart=f
 /
 &analyse max_ana=40 ana=t print=f nb_harm_ana=1 /
**
```

Active basis set

Inactive basis set (HADA)

Parameters for the effective Hamitonian on the active grid

test=t => the effective Ham is calculated on one grid point (reference geometry)

For the inactive namelist :

tab_nq(:) : number of grid points along each local normal modes (type 21)
tab_nb(:) : number of harmonic basis functions for each local normal modes
max_excit : enables to limit the numder of excitation (see NH3 parper)
max_ene_h : enables to limit the number nD-harmonic basis function (nD-HBF) (in cm-1)
sort : is true (default) the nD-HBF are sorted
n_h : number of coupled adiabatic channels used (can be lower than the number defined with the previous parameters, tab_nb, ….) when **non_adia=t** (cHADA)
n_h : when **non_adia=f**, one adiabatic channels is used (HADA). The number among the list generated whit tab_nb… is n_h

Remark: the local normal modes are built with the coordinates with 21 type (see Tnum data)
They are sorted with energy