```
#
# HCN with murell potential in 2D (angle + dHX)
#

 SYSTEM=sub_system_cos_hcn.f
 SYSTEM=sub_system_murrell.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
 /
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  1  0    0  0  0
 &minimum pot0=-0.499465823200 pot_act=f pot_cplx=f
          read_Qsym0=t read_nameQ=t unit='bohr' /
cosa .999d0
R 3.187
r 2.179
x 0.
pi 3.141592653589793238462643383279d0
dh 0.0
```

Do not those namelists

Definition of coordinates (zmatrix) as in Tnum

Here, the active variables are cos(a) and R, the other ones are rigid.

Definition of the reference energy pot0 and reference geometry.

pot_act=f, the coordinates of potential are not given in Qact order but Qsym order (here cos(a), R, r ...).

pot_cplx=f, if T, it uses the function im_pot0 (for CAP) in sub_system...f

read_Qsym0=t, coordinates are read in Qsym order.
read_nameQ=t, read the names of the coordinates (the names are not realy used).
unit='bohr', obvious. You can use unit='angs'.

Active basis set (here 2): see after for the different possibilities
iQact(1)=1 (basis associated with the first active coordinates
name: name of the basis set (Pl0: Legendre polynomial, boxAB: particle-in-a-box
nb : number of basis functions, **nq**: number of grid points

```
  "nD"    0    0   F    0     0. 1.
&basis_nD iQact(1)=1 name="Pl0" nb=51 nq=80 /
&basis_nD iQact(1)=2 name="boxAB" nb=20 nq=30 cte(1,1)=2.7 cte(2,1)=3.7 /


&inactives /



&actives test=f max_ene=20000.d0 lect=f
         non_adia=t restart=f
         direct=0
/
&analyse max_ana=40 ana=f print=f print_psi=50
         propa=f
/
**
```

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)

direct=0(1,2) : the matrix Hamiltonian is (not) build. direct=1,2 is used when the total number of basis functions is large (> 5000-10000).

propa=t => WP propagation, otherwise diagonalization

nD-Basis functions:

Primitive basis set (1D or 2D):

```
  Pl0       :    Legendre polynomials (in cos(theta))
  Pl0_0     :    id but only pair polynomials
  Pl0_1     :    id but only odd polynomials

  Pl0_a     :    Legendre polynomials (in theta)
  Pl0_a_0   :    id but only pair polynomials
  Pl0_a_1   :    id but only odd polynomials

  Hm        :    Hermite polynomials (Harmonic oscillator basis)
  Hm_0      :    id but only pair polynomials
  Hm_1      :    id but only odd polynomials

  cos or sin or fourier    :    fourier basis set ([-pi:pi])
  cosAB or cosABnosym      :    fourier basis set ([A:B])

  boxAB or boxABnosym      :    sine basis set (particle-in-a-box) ([A:B])

  Ylm       :    spherical harmonic basis set (2D basis set)
```

General basis set (up to 3D):

```
  direct_prod    : direct product basis set (up to 3D)
     You need to specify the other primitive or general basis-sets.
     It is only useful with contraction (nD).
See "dat_DirProd" example.
```