



# CARTE Half-Day: Hands On

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# Input file description



- FOUR blocks
  - `&path .... &end`
  - Optional
    - `&cartlist ... &end`
    - `&frozenlist ... &end`
  - Geometries
  - Input example [Gaussian, MOPAC]

# Input file description



- Main block: path
  - Only a few compulsory variables:
    - Nat: number of atoms
    - NgeomI: number of initial geometries
    - NgeomF: number of final geometries (including end points)

# Input file description



- Main block: path
  - Some important variables:
    - Prog: program used to compute the forces
    - PathOnly: if .TRUE. Path will only generate the initial path. Usefull to check that everything is fine: no atom reordering, ...
    - MaxCyc: Number of path optimization steps.
    - Ireparam: Frequency of the redistribution of the points along the path

# Tiny example



&path

nat=3, ! Number of atoms

ngeomi=3,! Number of initial geometries

nggeomf=12, !Number of geometries along  
the path

/

3

Energy : 0.04937364

H 0.0000 0.0000 0.0340

C 0.0000 0.0000 1.1030

N 0.0000 0.0000 2.2631

3

Energy : 0.04937364

H 0.0000 1.1000 1.1030

C 0.0000 0.0000 1.1030

N 0.0000 0.0000 2.2631

3

CNH

H 0.000000 0.000000 3.3

C 0.000000 0.000000 1.1

N 0.000000 0.000000 2.26

%chk=Test

#P AM1 FORCE

HCN est bien

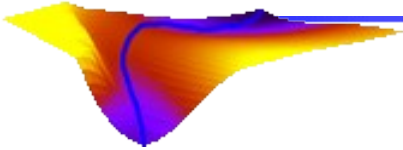
0,1

H 0.000000 0.000000 0.000000

C 0.000000 0.000000 1.000

N 0.000000 0.000000 3.00

# Tiny+ example



```
&path
nat=3, ! Number of atoms
ngeomi=3,
ngeomf=12,
PathOnly=.T., ! Only generate
initial path
```

```
/
```

```
3
```

```
Energy :    0.04937364
H   0.0000   0.0000   0.0340
C   0.0000   0.0000   1.1030
N   0.0000   0.0000   2.2631
```

```
3
```

```
Energy :    0.04937364
H   0.0000   1.1000   1.1030
C   0.0000   0.0000   1.1030
N   0.0000   0.0000   2.2631
```

```
3
```

```
CNH
H 0.000000   0.000000   3.3
C 0.000000   0.000000   1.1
N 0.000000   0.000000   2.26
```

```
%chk=Test
```

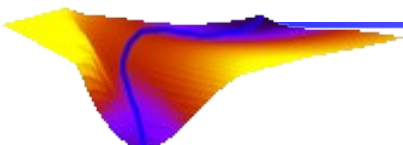
```
#P AM1 FORCE
```

```
HCN est bien
```

```
0,1
```

```
H 0.000000   0.000000   0.000000
C 0.000000   0.000000   1.000
N 0.000000   0.000000   3.00
```

# Tiny++ example



```
&path
nat=3, ! Number of atoms
ngeomi=3,
ngeomf=12,
Prog='test', !Use analytical PES for HCN
PathOnly=.F., ! Optimize the path
MaxCyc=10, ! Max number of iterations
```

/

```
3
Energy : 0.04937364
H 0.0000 0.0000 0.0340
C 0.0000 0.0000 1.1030
N 0.0000 0.0000 2.2631
```

3

```
Energy : 0.04937364
H 0.0000 1.1000 1.1030
C 0.0000 0.0000 1.1030
N 0.0000 0.0000 2.2631
```

3

```
CNH
H 0.000000 0.000000 3.3
C 0.000000 0.000000 1.1
N 0.000000 0.000000 2.26
```

# Tiny++ example: DIY

- Go to the Tiny directory:
  - cd CarteDay
  - cd Tiny
- Execute CARTE:
  - ./Path.exe Tiny++.path > Tiny++.out
  - ls

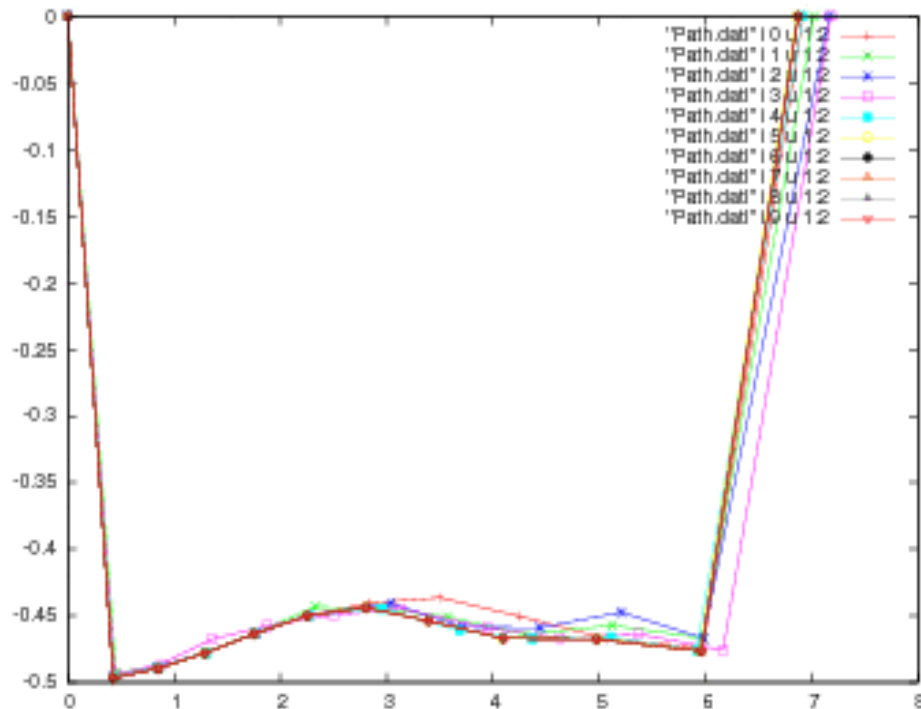
AnaPath

```
Path.1 Path.4 Path.7 Path_cart.0 Path_cart.3
Path_cart.6 Path_cart.9 Tiny++.out Tiny++.path list
Path.2 Path.5 Path.8 Path_cart.1 Path_cart.4
Path_cart.7 Path.exe Tiny.path Path.0 Path.3
Path.6 Path.9 Path_cart.2 Path_cart.5 Path_cart.8
Tiny+.path
```

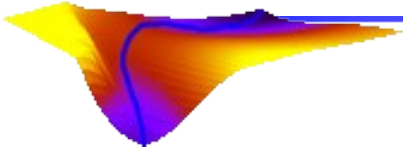


# Tiny++ example: DIY

- Analyse the path:
  - `./Anapath Tiny++.out 9 Path 12`
  - `./Path_12.gplot`



# Tiny2 example



```
&path
nat=3, ! Number of atoms
ngeomi=3,
ngeomf=12,
Ereac=-0.499465,
EProd=-0.481645,
Prog='test', !Use analytical PES for HCN
PathOnly=.F., ! Optimize the path
MaxCyc=10, ! Max number of iterations
/
3
Energy : 0.04937364
H 0.0000 0.0000 0.0340
C 0.0000 0.0000 1.1030
N 0.0000 0.0000 2.2631
```

3

Energy : 0.04937364

H 0.0000 1.1000 1.1030

C 0.0000 0.0000 1.1030

N 0.0000 0.0000 2.2631

3

CNH

H 0.000000 0.000000 3.3

C 0.000000 0.000000 1.1

N 0.000000 0.000000 2.26

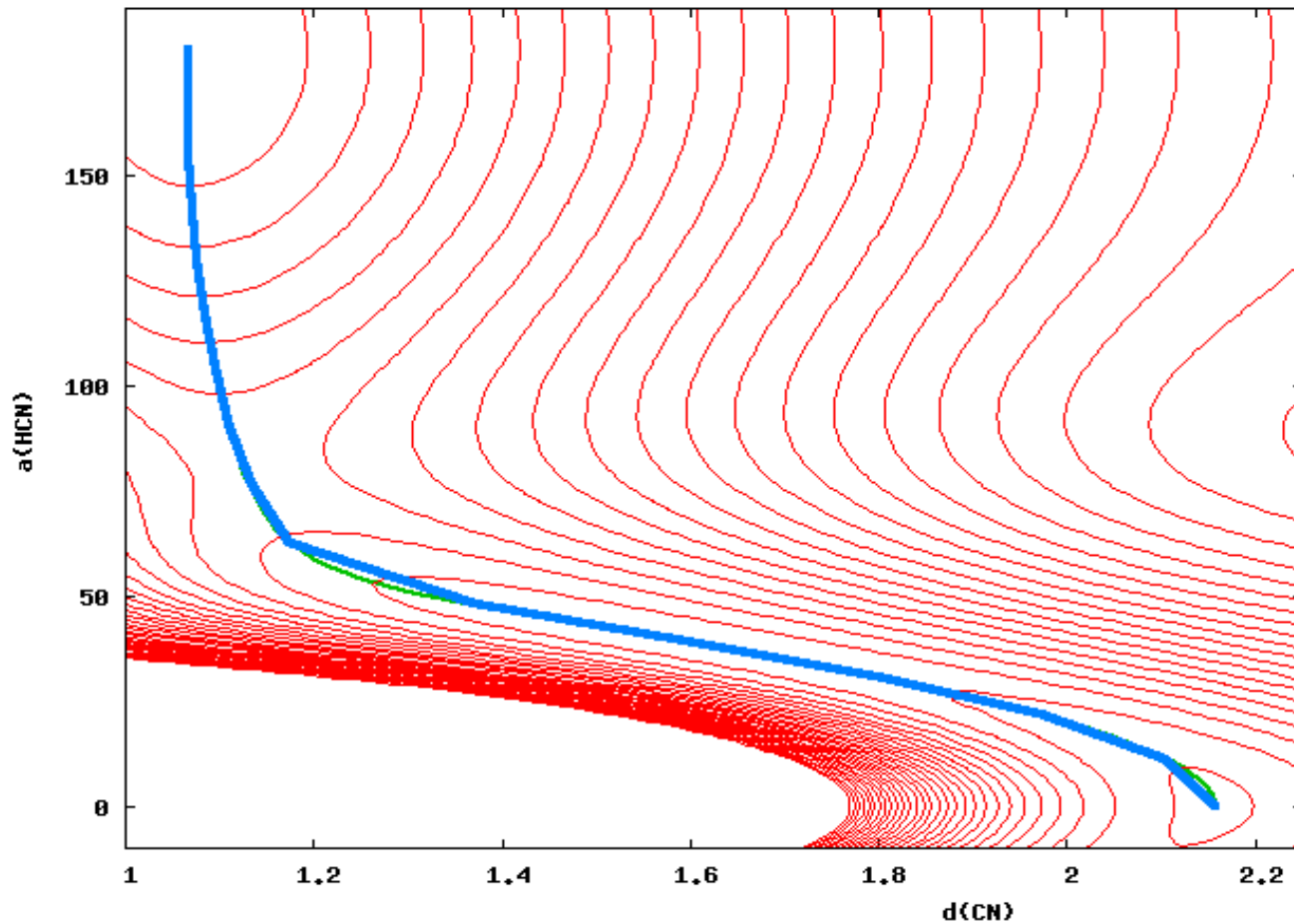
# Tiny2 example: DIY



- Modify Tiny++.paht into Tiny2.path
- Use Tiny2.path as input file
- Analyse the path:
  - `./Anapath Tiny2.out 9 Path 12`
  - `./Path_12.gplot`
- HCN is a special case, use `Dep_tscan_p`:
  - `./Dep_tscan_p Tiny2.out 9 Path PES`

# Tiny2 example: DIY

- `./Path_p.gplot`



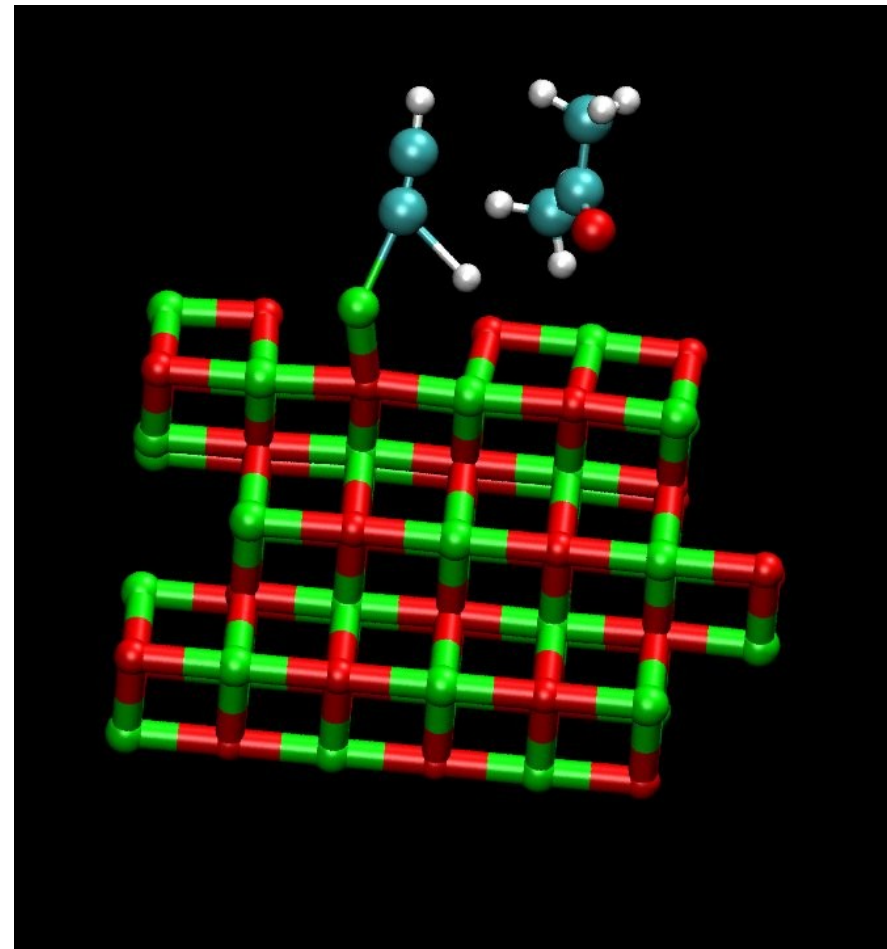
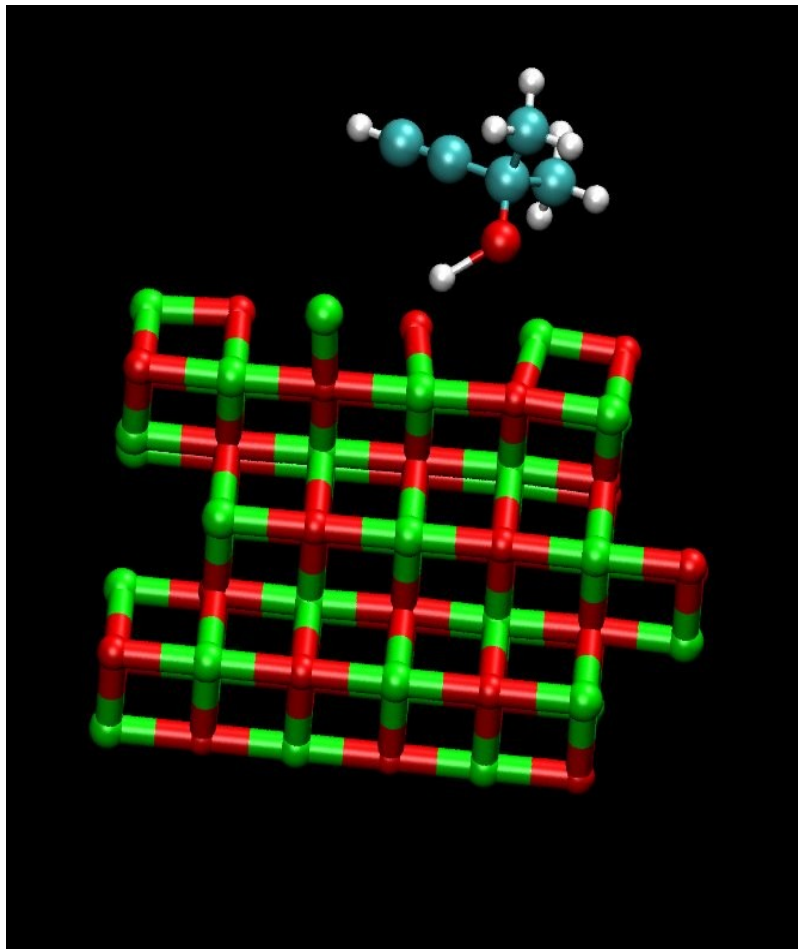
# Real example: more options



- What choices for the coordinates ?
  - Cart: cartesian
  - Zmat: Z-matrix
  - Mixed: Cart for some atoms, Zmat for others
  - Baker: Baker coordinates. Not yet efficient.
  - Hybrid: construct the path in Zmat, optimize it in Cart. See later.
- How important is the choice of the coordinates system ?

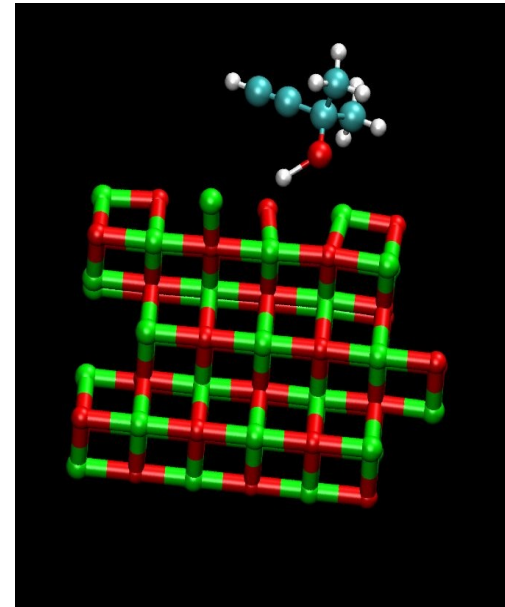
# Real example: more options

- Let us look at:



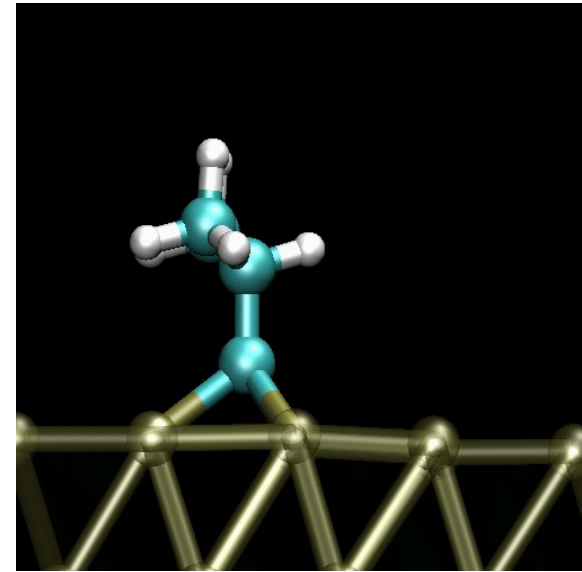
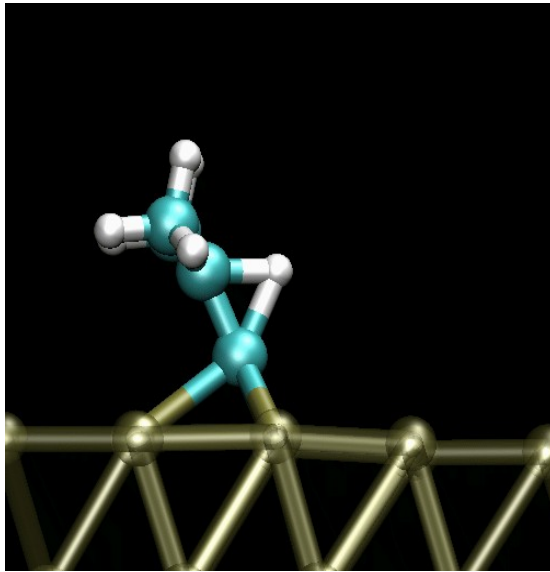
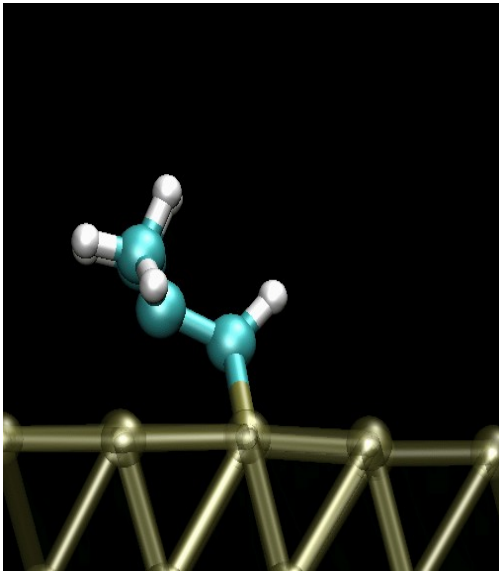
# Real example: more options

- Go to Hazar directory
- You will find: Hazar\_0.path
  - Prog='VASP'
  - Coord='Cart'
- Is the path ok ?
  
- Change into coord='mixed'
  - Better ?



# Real example: some troubles

- Let's play with the options of the 'mixed' coordinates



- Go to [TransferrH](#) directory



# Real example: some troubles



- Options for controlling the atoms:
  - Ffrozen: if **T**True, Path will look for a list of the frozen atoms in the `&frozenlist list=... &end` block.
  - Fcart: if **T**True, Path will look for a list of the cart atoms in the `&cartlist list=... &end` block.
  - Autocart: if **T**True, Path will analyse the geometries to decide which atoms should be described in `cart`.

# Real example: some troubles



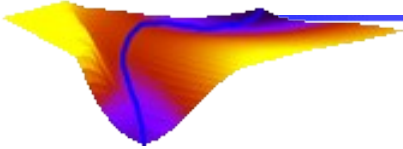
- Recommended strategy:
  - Use first `Autocart=T`, to see the guess of Path.
  - Analyse it to see if it is ok or not. Some usual cases:
    - Path is right, do not do anything. See Hazar example !
    - Path is wrong: some atoms are not cart and should be. Usually, it can improve the path to describe in cart an atom linked to other cart atoms...

# Real example: some troubles



- How to improve this path:
  - Use now `Autocart=F`, `Fcart=T` and add a `&cartlist list=...` `&end block`.
  - Try different lists of cart atoms and look at the differences.

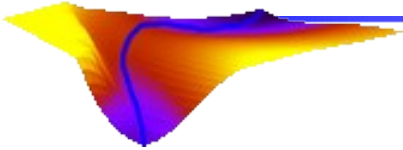
# Optimizing a path



- Recommended strategy:
  - Generate an initial path in 'Zmat' or 'mixed' coordinates with 32 images and `PathOnly=T`.
  - Typical input:

```
&path  
nat=XX,  
ngeomI=2, ngeomF=32,  
coord='mixed', pathonly=T, ...
```

# Optimizing a path



- Recommended strategy:
  - Use this first path as initial geometries for a cart optimisation
  - Typical input:

```
&path
```

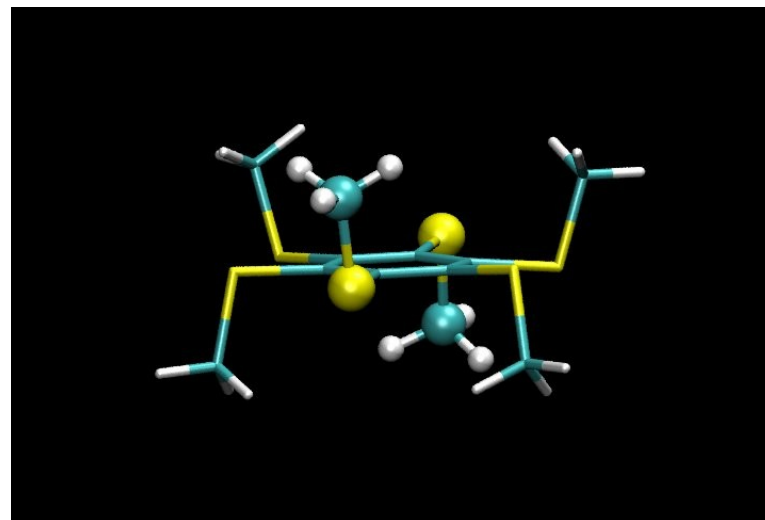
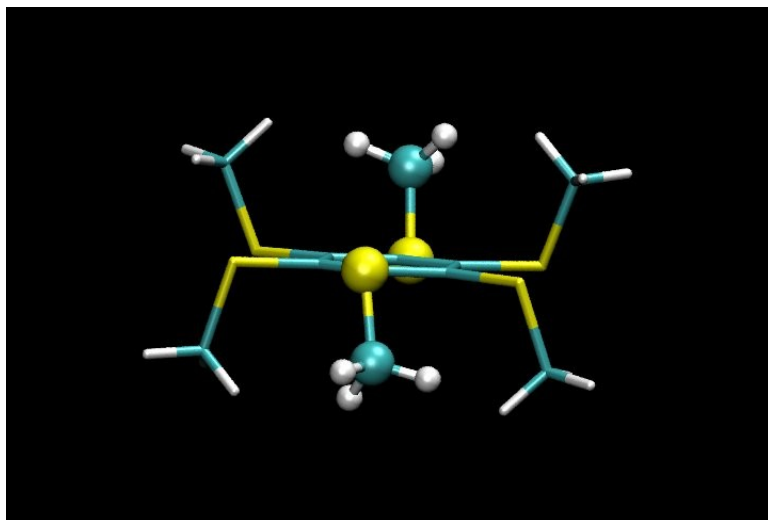
```
nat=XX,
```

```
ngeomI=32, ngeomF=10,
```

```
coord='cart', pathonly=F, ...
```

# Optimizing a path

- Example in CSR6:



- Note: In fact, interpolating in Zmat and optimizing in cart can be done at once using `cart='hybrid'`