EMORY Emerson Center for Scientific Computation

Reaction Profile of Pd(0) + 2 PH_3 + H_2

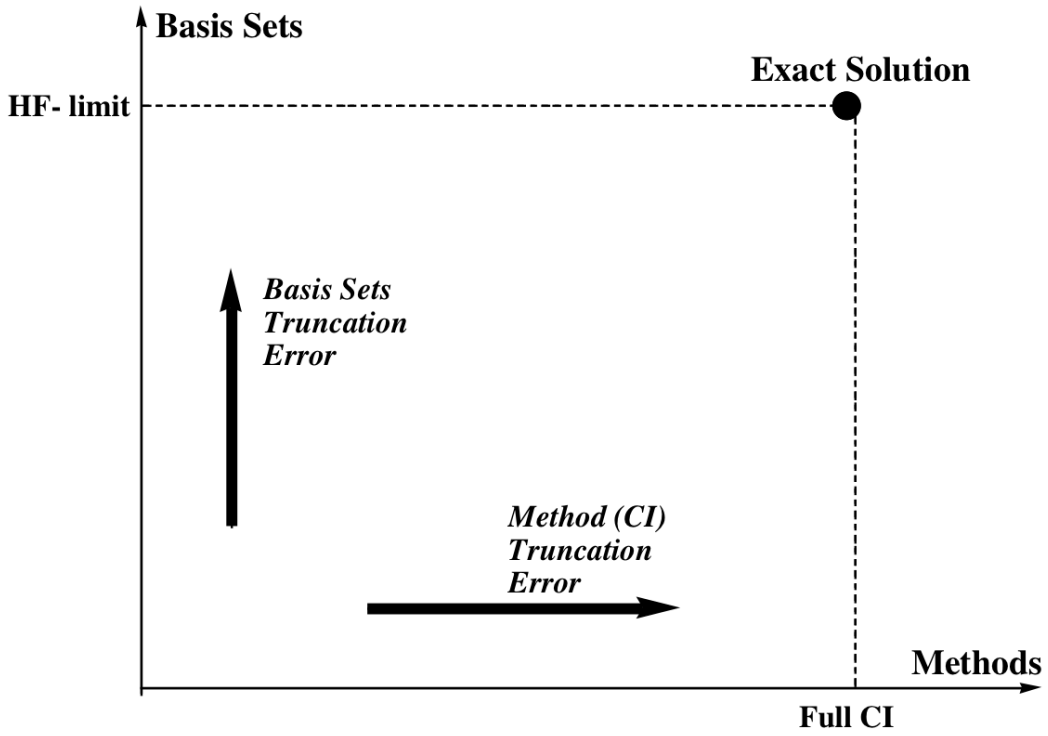
Practice Session

Quantum Chemical Calculations: What is necessary ?

method

$$H\Psi_I = E_I\Psi_I$$

Basis sets



Results are:

E_I Total Energy for state *I*

Ψ_I Wavefunction for state *I* is a probabilistic description of electronic motion for a given geometry, charge and spin state

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Command file (for LoadLeveler only):

```
#!/bin/ksh
#
###
# @ error = errcl.log
#
# @ initialdir = /star/chemistry/eclab/YOUR
# @ requirements = (Arch == "R6000") && (OpSys == "AIX53")
# @ notify_user = name@euch4e
# @ class = star16p
# @ group = ch_res
# @ queue
#
    INPF= test_inp
    OUTF= test_out

. /libs/scripts/g16/C01
chmod a+rw $OUTF
```

llsubmit xxxx.cmd

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Setting up Input for GAUSSIAN

Resource Section: **%chk, %nproc=16, %mem=@**

The route section:
Which kind of job you want to run: methods and basis sets.
Starts with a # sign **Opt, freq, pop=full etc.**

The title section: **ANY**

The Molecule specification section:
Charge on the molecule, Spin multiplicity**:** **0 1 or -1 1 or 1 1, etc**
Molecular structure (x,y,z coordinates)

Basis sets (if necessary)

Other Specific Requirements

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Practice Session

Pd(0)

H_2 molecule

$Pd(PH_3)_2$

$(H_2)Pd(PH_3)_2$

Transition State

$(H)_2Pd(PH_3)_2$

Pd-atom

```
%CHK=/starchk/chemistry/ch_res/eclab/jamal/pd_atom.chk
%nproc=16
%mem=24GB
#  b3lyp/gen empiricaldispersion=gd3bj pseudo=read optcyc=99
nosymm freq=noraman scf=xqc scfcyc=300

palladium_atom

 0 1
 Pd

Pd 0
lanl2dz
****

Pd 0
lanl2dz
```

H_2 MOLECULE

```
%CHK=/starchk/chemistry/ch_res/eclab/jamal/class_H2.chk
%nproc=16
%mem=24GB
#  b3lyp/gen empiricaldispersion=gd3bj optcyc=99 nosymm
   opt freq=noraman

H2- MOLECULE

 0 1
H
H 1 HH

 HH 0.75

H 0
6-31G(d,p)
****
```

$Pd^0(PR_3)_2$

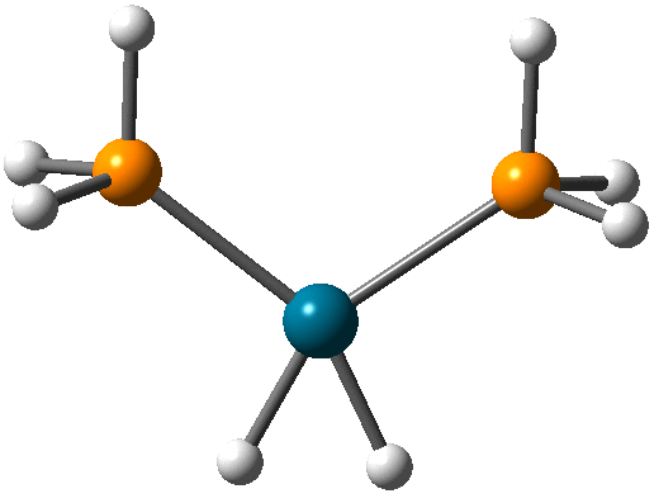
```
%CHK=/starchk/chemistry/ch_res/eclab/jamal/class_PdPH32.chk
%nproc=16
%mem=24GB
#  b3lyp/gen empiricaldispersion=gd3bj pseudo=read optcyc=99 nosymm
   opt freq=noraman

Title Card Required

 0 1
 Pd           -1.89777385    1.57389907    0.92659901
 P            -0.02304064    2.22509022    2.09577695
 P            -3.77846000    0.92160400   -0.24680000
 H            -3.83594400    1.04753800   -1.65796000
 H            -4.23811700   -0.41889300   -0.19850900
 H            -5.03863100    1.51995100    0.00715100
 H             1.10545636    2.75834122    1.42296695
 H            -0.09780964    3.23747122    3.08573995
 H             0.70053236    1.29704522    2.8868019

Pd 0
lanl2dz
****
H P 0
```

Transition state

1. Do freq=noraman calculation of rough Transition state structure
2. The first imaginary frequency should relate your reaction coordinate.
3. If so, read previously calculated frequencies and performed the opt=(ts noeig readfc).
4. At the optimized TS structure run the freq=noraman calculation, again

M = Pd: Transition State

ν_i = -643.58 cm^{-1}



IRC CALCULATIONS

5. Intrinsic Reaction Coordinate calculations from the optimized TS:

a. Forward: IRC=(RCFC forward maxpoint=@@) guess=read

b. Reverse: IRC=(RCFC reverse maxpoint=@@) guess=read

Run from TRUE transition state (with ONE imaginary frequency)