Cheatography

Gamess/Linux Keyboard Shortcuts

by [deleted] via cheatography.com/69782/cs/17672/

Linux commands

`cd`	Change directory
`mkdir`	Create directory
`rmdir`	Remove directory
`rm`	Remove file
`cp`	Copy file
`ls`	List of content of current directory

Exemple: `cp he.inp he3216.inp`

This will copy the file he.inp and rename the copy as he3216.inp

The studied atom/molecule

Multiplicity (n number of umpaired electron)	n+1(n number of umpaired electron)
Charge	+/-/0

Run gamess

`he.inp`	name of the input script
`he.out`	name of the output script
`rungms`	run gamess

Exemple : `rungms he> he.out`

Will run gamess with the script he.inp, and give you the output in the file he.out

Output file

How to see if my calculation worked?

> Look `density converged` in the output file

Where to see the final energy (HF) ?

> Right after the message `density converged` the Hartree Fock energy calculation is provided `FINAL RHF ENERGY IS=`

Where to see the final energy (MP2/CCSD) ?

> Look for a message `E(MP2/ CCSD)=`

How to see the number of basis fonction?

> Beginning of the output script there is a recap of the input script, and search for `Nb of cartesian basis fonction=`

⚠ RHF final energy is always provided even if you don't do HF calculation.

Input in $BASIS

STO-*n*G	`GBASIS=STO`	`NGA`
n-21G	`GBASIS=N21`	`NGA`
n-31G	`GBASIS=N31`	`NGA`
n-311G	`GBASIS =N311`	`NGA`
cc-PV*n*Z	`GBASIS=CC*n*`	! `I =1` i `TRC`
x shell polarisation function	`NxFUNC=number of set`	*x*=p
Semi empirical methods	`GBASIS =MNDO`	
	`GBASIS=AM1`	
	`GBASIS=PM3`	

Exemple:

- Calculation with 6-31G* Basis set for He

`GBASIS=N31 NGAUSS=6 NPFUNC=1`

- Calculation with 6-31G** Basis set for He

`GBASIS=N31 NGAUSS=6 NPFUNC=2`

Use P because He is full on s, not on p

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Input in $DATA

1. title/details
2. symmetry point group, usualy C1
3. empty line, unless symmetry different than C1
4. Atomic coordinates

▸ `COORDS =CART`

atome name / nuclear charge / X / Y / Z

```
H  1  0.0 0.0 0.0
C  6  1.1 0.0 0.0
```

▸ `COORDS=ZMT`

atom / I / distance / J / angle / K / torsion

```
H 1 1.1 2 125.0 3 180.0
```

▸ `COORDS =ZMTMPC`

atom / distance / 1 / angle / 1 / torsion / I / J / K

```
H 1.1 1 125.0 1 180.0 1 2 3
```

⚠ For `COORDS=ZMT` and `COORDS =ZMTMPC` , only put the required data !

Atom 1 : only name

Atome 2 : name + distance

Atome 3 : name + distance + angle

Atome 4 and + : all data

Input in $CONTRL

Method/Wave function choice	Close Shell System	`SCFTYP=RHF` default
	Open Shell System	`SCFTYP= UHF`
		`SCFTYP= ROHF`
		`SCFTYP=GVB`
		`SCFTYP= MCSCF`
Electron correlation method	Mollera-Plesseta MP*n*	`MPLEVL=n`
	DFT	`DFTTYP= word`
	coupled-cluster CC	`CCTYP= word`
	config-uration intera-ction CI	`CITYP= word`
	valence bond VB	`VBTYP= word`
	TDDFT	`TDDFT= word`

Input in $CONTRL (cont)

Other	Charge *n* of molecule	`ICHARG=n`
	Multiplicity *n* of molecule	`MULT=n`
	Format of geometry in `$DATA`	`COORDS= word`

DFT method's words: `VWN/BP 86/ BLYP...`

CC method's words: `CCD/CC SD/ CCS D(T)...`

Words for coordinates: `CART/Z MT/ ZMTMPC`

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