Lab2: Introduction to Gaussian16 software

Input and output files

- Input file extension: .gjf (gaussian job file) or .com
- Output file extension: .log

Input file

```
%nproc=N
%mem=XXGB
#HF/6-31G(d) SP


Title

Charge Multiplicity
Molecular coordinates (xyz format)

Additional input specifications
```

Input file

```
%nproc=N        !  Specifies the number of processors to be used.
%mem=XXGB       ! Allocates memory for the calculation
#HF/6-31G(d) SP! route section (method, basis set, calc type, and
additional keywords)

Title           ! A title for the job

Charge Multiplicity    !  The charge and multiplicity of the system.
Molecular coordinates (xyz format)    ! Cartesian coordinates of atoms

Additional input specifications
```

Input file - example

```
%nproc=4
%mem=8GB
#HF/6-31G(d) SP

Water optimization

0 1
O    0.000000    0.000000    0.000000
H    0.757160    0.586799    0.000000
H   -0.757160    0.586799    0.000000
```

How to create input file

- Use Avogadro 1.2 software
- Gaussview (commercial software)

Output file

Includes

- Initial system information.
- SCF (Self-Consistent Field) iterations and convergence details.
- Final atomic coordinates.
- Electronic structure information, including orbital energies.
- Charges, dipole moment, etc
- Total energy and thermodynamic properties.
- Vibrational frequencies for vibrational analysis.
- etc.

Output file

Includes

- Initial system information.
- SCF (Self-Consistent Field) iterations and convergence details.
- Final atomic coordinates.
- Electronic structure information, including orbital energies.
- Charges, dipole moment, etc
- Total energy and thermodynamic properties.
- Vibrational frequencies for vibrational analysis.
- etc.

Input file

```
%nproc=N        !  Specifies the number of processors to be used.
%mem=XXGB       ! Allocates memory for the calculation
#HF/6-31G(d) SP! route section (method, basis set, calc type, and
additional keywords)

Title           ! A title for the job

Charge Multiplicity    !  The charge and multiplicity of the system.
Molecular coordinates (xyz format)    ! Cartesian coordinates of atoms

Additional input specifications
```

Input file

```
%nproc=N        !  Specifies the number of processors to be used.
%mem=XXGB       ! Allocates memory for the calculation
```

- Multi Node job not allowed unless license permits
- Number of cores should be given based on the parallelization capabilities of the QM method
- OpenMP thread parallel model
- Sufficient memory should be given to avoid job crashes or slowness

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Methods are generally categorized into four,

- Semiempirical: PM6, ZINDO, AM1, etc
- Ab initio: HF, MPn, etc
- Density functional theory: B3LYP, M06L, etc
- Molecular mechanics: GAFF, MMFF6, UFF, etc

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Basis sets

- Minimal: STO-3G, etc
- Split valence: 6-31G, 6-311G, 6-31G(d)/6-31G*, 6-31+G(d), etc
- Correlation-consistent: cc-pVDZ, aug-cc-pVDZ, etc
- Def2-basis sets: Def2-SVP, Def2-TZVPP, etc

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: Single point energy

- Single point energy in Hartree or atomic unit
- Orbital symmetries
- Mulliken atomic charges
- Dipole moment

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: Geometry optimization or energy minimization

- Final atomic coordinates and the corresponding energy
- Bond lengths, angles, etc
- HOMO/LUMO eigenvalues
- Mulliken atomic charges
- Dipole moment

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: Population analysis

- Partial atomic charges
- Dipole moment

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: UV/Visible and vibronically-resolved electronic spectra

- Ground to excited state transition
- Excitation energies and oscillator strengths
- Electronic Circular Dichroism (ECD)

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: Solvation

- Energy, atomic charges, dipole moments, etc
- Final atomic coordinates if optimization is selected
- Vibrational analysis and thermochemistry

Input file

```
#HF/6-31G(d) SP! route section (method, basis set, calc type, and additional keywords)
```

Calc type: Scan, Transition state optimization

- Energy, atomic charges, dipole moments, etc
- Transition states, reaction energies

Molecular properties available in Gaussian 16

- Antiferromagnetic coupling
- Atomic charges
- ΔG of solvation
- Dipole moment
- Electron affinities
- Electron density
- Electronic circular dichroism (ECD)
- Electrostatic potential
- Electrostatic potential-derived charges
- Electronic transition band shape
- High accuracy energies
- Hyperfine coupling constants (anisotropic)
- Hyperfine spectra tensors (including g tensors)
- Ionization potentials
- IR and Raman spectra*
- Pre-resonance Raman spectra*
- Resonance Raman spectra
- Molecular orbitals
- Multipole moments
- NMR shielding and chemical shifts
- NMR spin-spin coupling constants
- Optical rotations (ORD)
- Polarizabilities/hyperpolarizabilities
- Raman optical activity (ROA)*
- Thermochemical analysis
- UV/Visible spectra
- Vibration-rotation coupling
- Vibrational circular dichroism (VCD)*
- Vibronic (absorption and emission) spectra

*Harmonic approx. and including anharmonic effects

Run your first calculation in gaussian software

User accounts: cd61006-g1, ... , cd61006-g8

IP addr: 10.171.16.243

Do not use more than 4 cores per job

Do not run more than 1 job at any moment

References

1. https://avogadro.cc/
2. https://gaussian.com/gaussian16/
3. https://zipse.cup.uni-muenchen.de/teaching/computational-chemistry-1/topics/