

Instructions for Submitting Jobs on OSACA (CY Cergy Paris University)

Step 1:

Open a terminal and execute the following command, then press Enter:

```
ssh user@osaka.cyu.fr
```

(Replace 'user' with your actual username.)

Step 2:

You will be prompted to enter your password. Type your password and press Enter.

Step 3:

You are now logged in to osaka.cyu.fr.

Step 4:

Prepare the following input file named test.inp:

```
!PBE D4 DEF2-SVP OPT
```

```
%maxcore 4000
```

```
%pal
```

```
nprocs 8
```

```
end
```

```
* xyz 0 1
```

```
N   -0.83911    0.76325   -0.31843
```

```
C    0.61442    0.72014   -0.25075
```

```
C    1.01669   -0.56167    0.49740
```

```
O    0.20095   -1.36984    0.93753
```

```
H   -1.37884    0.05803    0.17605
```

```
H    1.00414    0.66192   -1.27362
```

```
C    1.17285    1.95192    0.45211
```

```
H    0.87124    2.87150   -0.05988
```

```
H    0.81191    2.01288    1.48492
```

```
H    2.26726    1.92903    0.48485
```

```
H   -1.30551    1.57618   -0.71069
```

```
O    2.33980   -0.77979    0.66176
```

```
H    3.04559   -0.08055    0.28096
```

```
*
```

Step 5:

Create the following job submission script and save it as sub.sh:

```
#$ -N test
#$ -l m_mem_free=32G
#$ -pe openmp 8
#$ -cwd
# This is a comment
```

```
module load orca/6.0.1
module load openmpi/5.0.5
```

```
/usr/local/orca/6.0.1/orca test.inp > test.out
```

Step 6:

Ensure that both test.inp and sub.sh are in the same directory. Then submit the job by running the following command:

```
qsub sub.sh
```

Step 7:

The job is now submitted to the queue. To check the status of your job, type:

```
qstat
```

Step 8:

The output of the calculation will be written to the file test.out.