CMMDE: An Introduction to Three New Features in ORCA 6

By CMMDE Core Team

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August 17, 2024

Outline

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CMMDE: Computational Molecular and Material Design Environment

Why did we develop CMMDE?

CMMDE was developed to reduce the difficulties of preparing input files and analyzing popular computational chemistry software outputs.

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What CMMDE can do

- Preparing the input files
- Submitting the calculations to the queueing system (if available)
- Analyzing the outputs

Outline

Implicit Solvations in Orca 6

Currently supported solvation models

- ALPB (only for XTB calculations at `GFNFF`,`GFN0XTB`, `GFN1XTB`, and `GFN1XTB` levels)
- GBSA (Also for XTB)
- CPCM
- Cosmo-based CPCM (CPCMC)
- SMD
- SMD with DRACO

Implicit Solvation in CMMDE (ammonia in water)

```
cmmde.py -i "N" -j opt -solvent water -solvtype GBSA
```

Implicit Solvation in CMMDE (Cont'd)

If we want to use other solvation models

```
cmmde.py -i "N" -j opt -solvent water -solvtype SMD
cmmde.py -i "N" -j opt -solvent water -solvtype CPCM
cmmde.py -i "N" -j opt -solvent water -solvtype CPCMC
```

If we want to activate the DRACO model

```
cmmde.py -i "N" -j opt -solvent water -solvtype SMD
-draco True
```

A Hybrid of Explicit and Implicit Solvation

Glucose solvated by 10 water molecules

```
cmmde.py -i "C(C1C(C(C(C(O1)O)O)O)O)O" -solvent water
-solvator true -nsolv 10
```

- Currently, the solvator module can only handle the ALPB solvation model.

Reoptimizing the solvation structure

```
cmmde.py -i cmmd.solvator.solventbuild.xyz -j opt -m
XTBFF -solvent water
```

- Alternative methods (`-m`): `GFN0XTB`, `GFN1XTB`, and `GFN2XTB`.

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Docker: A Quantum Mechanical Docking

- The docker module can automate the binding pocket search through three levels of accuracy:
  - `SCREENING`: A low accuracy docking, good for a larger dataset for an initial screening process.
  - `NORMAL`: A moderate accuracy docking, with a moderate level of accuracy. It is good for a medium-size dataset.
  - `COMPLETE`: A robust docking with a higher level of accuracy, only for the screening of a very small dataset.

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General CMMDE command for Orca6's docker

```
cmmde.py -j docker -i host.xyz -guest guest.xyz
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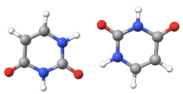
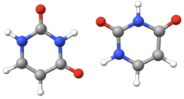
For an arbitrary run, you can change the host and guest molecules above.

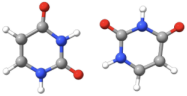
Example 1: Uracil Dimerization



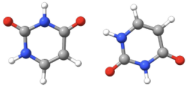
6
(0.0 kcal/mol)



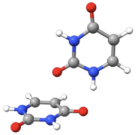
9
(2.9)



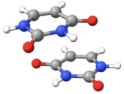
4
(4.0)



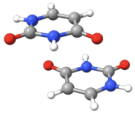
2
(5.6)



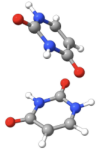
1
(6.8)



11
(8.0)



3
(8.6)



10
(11.1)

```
cmmde.py -j docker -i uracil.xyz -np 8 -guest uracil.xyz
```

Example 1: Uracil Dimerization (Cont'd)

Step 1: Geometry Optimization

- `mkdir uracil; cd uracil`
- `cmmde.py -j opt -i "C1=CNC(=O)NC1=O" -np 8`

Example 1: Uracil Dimerization (Cont'd)

Step 1: Geometry Optimization

- `mkdir uracil; cd uracil`
- `cmmde.py -j opt -i "C1=CNC(=O)NC1=O" -np 8`

Step 2: Docking

- `cd ../; mkdir UracilDimer; cd UracilDimer`
- `cmmde.py -j docker -i ../uracil/cmmd.xyz -guest ../uracil/cmmd.xyz -np 8`

- **Running time: 4 minutes 18 seconds 32 msec**
- Important message from the output: `LOWEST INTERACTION ENERGY: -18.481342 kcal/mol (structure 9)`

Example 2: Li-ion Binding Sites in Glucose

Step 1: Make a simple Li-ion Cartesian

- `mkdir li; cd li`
- `echo -e "1 \n \nLi 0 0 0" > geom.xyz`

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Step 2: Geometry Optimization of Glucose

- `cd ../;mkdir glucose;cd glucose`
- `cmmde.py -j opt -i "O[C@@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@]([H])(CO)O1" -np 8`

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Example 2: Li-ion Binding Sites in Glucose (Cont'd)

Step 3: Docking

- `cd ../; mkdir GlucoseLi3; cd GlucoseLi3`
- `cmmde.py -j docker -i ../glucose/cmmd.xyz -guest ../li/geom.xyz -guestcharge 1 -nrepeat 3 -np 8`

- `-nrepeat 3`: Herein, three lithium ions will be coordinated to the active sites of the glucose.
- `-guestcharge 1`: The charge of lithium-ion is $+1$.
- Important outputs:
  - `cmmd.docker.struc1.allopt.xyz`: Glucose + 1 Li^+
  - `cmmd.docker.struc2.allopt.xyz`: Glucose + 2 Li^+
  - `cmmd.docker.struc3.allopt.xyz`: Glucose + 3 Li^+
  - `cmmd.docker.xyz`: The best structure

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Example 1: Cyclohexane Conformation

Step 1: Geometry optimization of cyclohexane

- `mkdir cyclohexane; cd cyclohexane`
- `cmmde.py -j opt -i "C1CCCCC1" -np 8`

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- `mkdir cyclohexane; cd cyclohexane`
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Step 2: Global optimization of Cyclohexane

- `cd ../; mkdir GOATcyclohexane; cd GOATcyclohexane`
- `cmmde.py -j goat -i ../cyclohexane/cmmd.xyz -np 8`

Example 2: Oxidation of Glucose

Step 1: Geometry optimization of O_2

- `mkdir oxygen;cd oxygen`
- `cmmde.py -j opt -i "O=O" -mult 3 -np 8`

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Step 1: Geometry optimization of O_2

- `mkdir oxygen;cd oxygen`
- `cmmde.py -j opt -i "O=O" -mult 3 -np 8`

Step 2: Docking

- `cd ../; mkdir GlucoseOxygen; cd GlucoseOxygen`
- `cmmde.py -j docker -i ../glucose/cmmd.xyz -guest ../oxygen/cmmd.xyz -m XTBFF -np 8`

Example 2: Oxidation of Glucose (Cont'd)

Step 3: Prediction of glucose oxidation products

- `cd ../; mkdir REACTGlucoseOxygen; cd REACTGlucoseOxygen`
- `cmmde.py -j GOAT-REACT -i ../GlucoseOxygen/cmmd.docker.xyz -gfn_up GFN1XTB -np 8`

Thank You!

By CMMDE Core Team

- Aditya Wibawa Sakti
- Muhamad Abdulkadir Martoprawiro
- Atthar Luqman Ivansyah
- Nova Pratiwi Indriyani
- Eduardus
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- Rustaman
- Mirella Fonda Maahury
- Hasan Al-Rasyid
- Arifin
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