SICTWO V1.0

Manual

Shell Interface for Combining Tinker with ONIOM (SICTWO)

by

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1. Introduction

This manual provides a quick guide to the Shell Interface for Combining Tinker with ONIOM (SICTWO) program. SICTWO gives access to the force fields in the Tinker program from Gaussian09 (or Gaussian16) calculations. The ONIOM(QM:MM) implementation in SICTWO supports for the polarizable and non-polarizable force fields in the TINKER program;

---AMOEBA polarizable atomic multipole force field
---Liam Dang's polarizable model
---AMBER
---CHARMM
---MM2 (1991), MM3 (2000)
--- OPLS
---Merck Molecular Force Field (MMFF)
etc.

SICTWO does not require modifications to either the Tinker or Gaussian09/16 original codes. SICTWO program can be obtained from the authors.

2. How to install SICTWO

Step 1

Gaussian09/16 and tinker must be installed in your system.

Step 2

Place the `sictwo_files.tar` file in your working directory. Then, extract the *tar* file, copy the `sictwo_files` directory into your working directory, from where you are going to submit the calculations. All SICTWO modules are collected in this directory. All files in the directory must have execution permission.

Step 3

Modify the path for the $GAUSS_SCRDIR directory in the `sictwo` and `sictwo_g09d01` modules. This modification must be applied into two places;

```
#
# Add the full path for the Gaussian09 scratch directory, $GAUSS_SCRDIR
#
cp $GAUSS_SCRDIR/*.EIn .
#
```

and

```
#
# Add the full path for the Gaussian09 scratch directory, $GAUSS_SCRDIR
#
cp inp.EOu $GAUSS_SCRDIR/$checkEOu
#
```

Step 4

Prepare files for Tinker execution.

Copy the `analyze`, `testgrad`, and `testhess` modules of Tinker to the `sictwo_files` directory. These files are typically located in the bin directory of the Tinker installation tree.

Prepare `inp.par` and `mm.type` files for the calculation. Follow the instructions below concerning each module.

Step 5

Prepare the Gaussian09 input file. The `sictwo` module can be activated by including the `external="./sictwo_files /sictwo"` keyword in your Gaussian09 input file. If you use Gaussian09 Rev.D01 version or Gaussian16, assign the `external="./sictwo_files/ sictwo_g09d01"` keyword.

After these steps, SICTWO is ready to use. You can submit the Gaussian09 job as a regular calculation. SICTWO will generate several intermediate files in the `sictwo_files` directory, and these files will be removed at the end of the calculations.

There are few examples can be found in the `sictwo_files/examples` directory.

Note: You cannot use a common `sictwo_files` directory to run two (or more) calculations simultaneously. If necessary, you can create `sictwo_files2`, `sictwo_files3`, etc.

3. Overall structure of the interface

The operating mechanism of the SICTWO interface and its modules are summarized in Figure 1. SICTWO needs access to the Gaussian09 (or Gaussian16) and Tinker codes. Gaussian 09 licenses can be obtained from Gaussian Inc. Tinker program can be downloaded from Tinker home page.

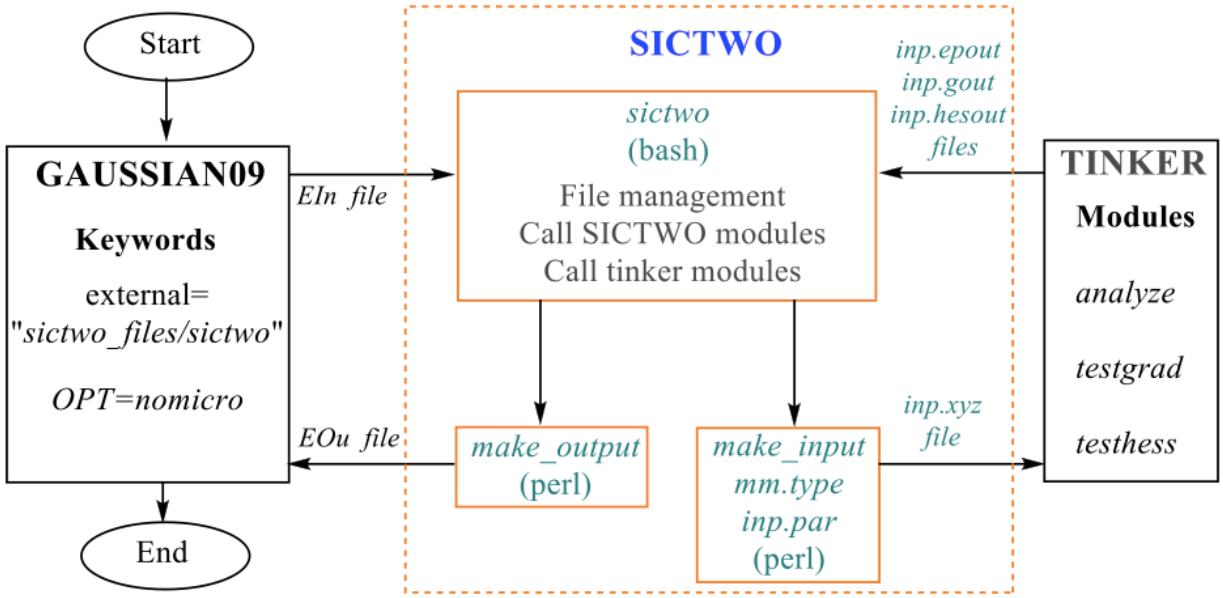

Figure 1. Overall mechanism of SICTWO interface between the Gaussian09 and Tinker programs.

The modules of SICTWO can be obtained from the authors. All modules are collected in the "`sictwo_files`" directory, and this is kept in the working directory. The `sictwo` module of SICTWO program can be executed by using the `external="sictwo_files/sictwo"` keyword in the Gaussian09 input file. Then, SICTWO performs the following tasks; (i) transforms the information in the Gaussisn09 `EIn` file into a format suitable for the Tinker program, (ii) converts MM atom types for Tinker, (iii) calls different Tinker modules to carry out the MM calculation, and (iv) transforms the Tinker outputs into a format suitable for Gaussian09 (a file with the `EOu` extension). Gaussian09 recovers MM energy and derivatives, and continues the operations, such as single-point, geometry optimization, frequency calculation, etc.

4. Modules of SICTWO

This section provides information about the modules of SICTWO. All modules can be can be obtained from the authors. The program consists of several scripts; `sictwo`,

`sictwo_g09d01`, `make_input`, `make_input_g09d01`, `make_output`, `inp.par`, and `mm.type`. Most of them should not be modified in everyday work by the user, with the exception of two: `inp.par` and `mm.type`.

4.1 `inp.par` file

The `inp.par` file contains full path for the Tinker force field parameter files (prm). The force field may be directly taken from the Tinker directory tree, typically in `$tinker/install_dirs/params`. For a different force field, one should modify the corresponding line.

The `inp.par` can also be modified to include a wide variety of switches (for the user familiar with MM or Tinker) and introduce missing potential parameters in this file. A sample `inp.par` file is shown below;

```
# ******************************************************
#    Path for the TINKER force field parameter file
# ******************************************************
#
parameters mm3
#
# ******************************************************
#    Define missing potential parameters
# ******************************************************
#
# Missing atoms
#
atom   165   X   "Os atom"   76   190.23   4 # X is Os
# Missing VWD parameters
#
vwd    165   0.037   1.560
#
# Missing bond parameters
bond   7   165   0.3     1.67
#
# Missing bond angle parameters
angle   7   165  7    0.5     90.0
#
# Missing torsion parameters
torsion  2  1  6  2   0.0  0.0  1  0.0  180.0  2  0.403 0.0  3
#
```

4.2 mm.type file

The mm.type file of SICTWO consists of atom type conversions between Gaussian09 and Tinker, and this section has to be defined by user. Depending on the force field of interest, user can keep separate mm.type files. Eg: amber96.type, charmm19.type, mm3.type, oplsaa.type, amoeba09.type, etc.

This file is fundamental for the calculations, and is likely to require specific modifications for almost each family of calculations. This file contains the information to map the atom-types in the Gaussian09 input file, which must be UFF, AMBER or Dreiding, into the atom-types in the Tinker program, which are associated to the corresponding force field.

The construction of this file is the most likely source of trouble for the user. Because of this, we discuss more details here.

The general format of the script for atom type conversions is;

```
# if($atom[$lnum] eq "G09 atom type") {$atomc[$lnum] = "TINKER atom type"};
```

You can fill the "G09_atom_type" section of above script with the UFF, AMBER or Dreiding atom types from the Gaussview software. Detailed information about the UFF, AMBER or Dreiding atom types can be found in the literature. Corresponding TINKER atom types go to the "TINKER_atom_type " section, where you can check the MM parameter files (prm) of Tinker home directory and select the suitable atom types. A sample Perl script for UFF -> MMFF atom type conversion is shown below;

```
# Following format is required
# if($atom[$lnum] eq "G09_atom_type") {$atomc[$lnum] = TINKER_atom_type};
#
if($atom[$lnum] eq "C_3") {$atomc[$lnum] = 1};
if($atom[$lnum] eq "C_R") {$atomc[$lnum] = 3 };
if($atom[$lnum] eq "H_") {$atomc[$lnum] = 23};
if($atom[$lnum] eq "S_R") {$atomc[$lnum] = 148 };
if($atom[$lnum] eq "O_3") {$atomc[$lnum] = 41 };
#
#
```

Notes:

User would define atoms types for "G09_atom_type" in the Gaussian09 input in the following cases;

1. If you find more than one TINKER atom types for an atom of your molecule.
Let´s assume one of the hydrogen atoms in your molecule is an amide hydrogen. Gaussview prints "H-H_" symbol for all hydrogen atoms including the amide hydrogen, where UFF atom type is "H_". In order to use the amide hydrogen in the Tinker force field, you can introduce "H_A" (or any other symbol) for G09_atom_types of the amide atom to "H_A" (or any other symbol) in the mm.type file;

```
# Convert atom type for hydrogen
   if($atom[$lnum] eq "H_") {$atomc[$lnum]  = 1};
#
# Convert atom type for amide hydrogen
   if($atom[$lnum] eq "H_A") {$atomc[$lnum] = 28};
#
```

2. In order to minimize the problems associate with Gaussian09 EIn files, we recommend you to keep three (or less) characters for the "G09_atom_type". For instance, let´s assume that you have an Os ion in your system. Gaussview sets "Os-Os6+6" in the input file, where "Os6+6" is the UFF atom type, which you can change into a different character, such as "X" as shown in the following mm.type file;

```
#
# Convert atom type of Os
   if($atom[$lnum] eq "X")   {$atomc[$lnum] = 165}; # X is Os
#
```

3. The Molden software can be used to generate Tinker force field atom types (E.g. MM3). Further, open your molecule (or complex) with Molden and assign a Tinker force field in the "Atom Attributes Window". Then, you can save your molecule as a Tinker Cartesian coordinates file (xyz), which may report TINKER atom types of your molecule. Moreover, the first line of the file contains the number of atoms followed by the title line. Then, molecular structure is defined, where each line contains the sequential number within the structure, an atomic symbol, X-, Y-, and Z-coordinates, the force field atom type number of the atom, and a list of the atoms connected to the current atom. Sample Tinker Cartesian coordinates file is shown below;

```
8    Ethane
1   C    0.000000    0.000000    1.455089   1   2   3   4   5
2   H   -0.951581    1.651885    2.129090   5   1
3   H   -0.954783   -1.650036    2.129090   5   1
4   H    1.906365   -0.001848    2.129090   5   1
5   C    0.000000    0.000000   -1.455089   1   1   6   7   8
6   H    0.954783   -1.650036   -2.129090   5   5
7   H   -1.906365   -0.001848   -2.129090   5   5
8   H    0.951581    1.651885   -2.129090   5   5
```

The Tinker force field atom types that Molden generates may be not accurate. Therefore we recommend you to compare them with the force field atom types in the Tinker *prm* files. As an additional test, you can use above Tinker Cartesian coordinates file to execute `analyze` module of Tinker, which provides information about your molecule (you need Tinker key file for this execution - refer Tinker user manual for more details). Normal termination of this execution indicates your atom type assessment is correct.

4. If the missing parameters correspond to the atoms in the QM region, you may take them from the UFF (or other force field) parameters. If you follow this option for the atoms in the MM region, we strongly suggest you to check the optimized structures very carefully. E.g. if you are using OPLSAA, you may obtain missing parameters from GROMACS. For transition metals, you may be able to use missing parameters from the universal fore field (UFF). *All these choices concerning parameters must be reported when presenting results, so other authors can reproduce your calculations.*

5. Examples

The last section of this manual presents few examples for application of SICTWO.
Note: We have used TINKER 7.1 version for MM calculations. If you use a different version, TINKER atom types may be different.

Ex1: RESVAN system: ONIOM(B3LYP:MMFF) optimization. *(QM: Gaussian09 Rev.A02, MM:Tinker 7.1) version.*

This section uses RESVAN system (Figure 2) to illustrate the key steps to setup an ONIOM(DFT:MM3) calculation.

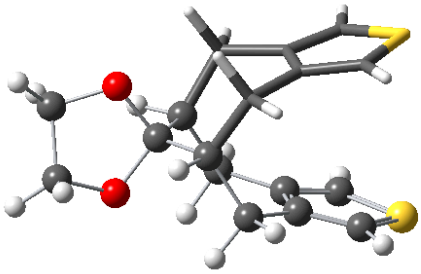

Figure 2. QM/MM molecular model of RESVAN system ('ball and stick' model represents the QM region and 'tube' model represents the MM region).

Step 1

We assume that the Gaussian09 and Tinker programs are installed in your computer system. Use Gaussview software to set up your ONIOM(B3LYP:MMFF) calculation, where you can refer Figure 2 to select the QM and MM partitions. Assign UFF parameters for the MM part. We are going to script UFF → TINKER atom types conversion in Step 2. Copy this input file (E.g. resvan.in) into your working directory.

```
%nprocshared=8
%mem=8000MB
%chk=test
#p opt=nomicro oniom(B3LYP/TZVP:external="./sictwo_files/sictwo")
geom=connectivity nosymm scf(maxcyc=100)

ONIOM(QM:MM) OPT FREQ with SICTWO V1.0

0 1 0 1 0 1
 S-S_R                0    2.93200000   -2.05800000   -0.05500000 H
 S-S_R                0    3.02700000    1.85800000    0.11400000 L
 O-O_3                0   -3.02800000   -1.09900000   -0.12100000 H
 O-O_3                0   -2.97300000    1.19800000    0.00800000 H
 C-C_3                0   -2.13500000    0.02800000   -0.04400000 H
 C-C_3                0   -1.37600000   -0.05200000    1.28600000 H
 H-H_                 0   -2.16600000   -0.06600000    2.07800000 H
 C-C_3                0   -0.59700000   -1.36300000    1.47800000 H
 H-H_                 0   -0.27800000   -1.42300000    2.54400000 H
 H-H_                 0   -1.28200000   -2.22800000    1.33000000 H
 C-C_R                0    0.62000000   -1.57700000    0.60100000 H
 C-C_R                0    1.83300000   -1.86800000    1.09300000 H
 H-H_                 0    2.05900000   -1.97200000    2.16500000 H
 C-C_R                0    1.87300000   -1.76100000   -1.21800000 H
 H-H_                 0    2.13400000   -1.76500000   -2.28600000 H
 C-C_R                0    0.64300000   -1.51500000   -0.74100000 H
```

```
C-C_3                0   -0.54400000   -1.21900000   -1.63600000 H
H-H_                 0   -1.23100000   -2.09500000   -1.59300000 H
H-H_                 0   -0.18800000   -1.18000000   -2.69200000 H
C-C_3                0   -1.33500000    0.06800000   -1.35100000 H
H-H_                 0   -2.10000000    0.12100000   -2.16600000 H
C-C_3                0   -0.48600000    1.33900000   -1.52000000 L H-H_ 20
H-H_                 0   -0.13400000    1.38300000   -2.57700000 L
H-H_                 0   -1.13200000    2.23700000   -1.39100000 L
C-C_R                0    0.71400000    1.49300000   -0.60800000 L
C-C_R                0    1.95400000    1.72300000   -1.06600000 L
H-H_                 0    2.21500000    1.81400000   -2.13100000 L
C-C_R                0    1.92100000    1.61600000    1.24600000 L
H-H_                 0    2.15200000    1.60700000    2.32100000 L
C-C_R                0    0.69500000    1.43100000    0.73400000 L
C-C_3                0   -0.53000000    1.19500000    1.59400000 L H-H_ 6
H-H_                 0   -1.17100000    2.10400000    1.53200000 L
H-H_                 0   -0.20700000    1.13900000    2.65900000 L
C-C_3                0   -4.31300000   -0.60700000    0.23100000 H
H-H_                 0   -4.42600000   -0.57300000    1.33400000 H
H-H_                 0   -5.11000000   -1.24600000   -0.19700000 H
C-C_3                0   -4.27000000    0.77000000   -0.38100000 H
H-H_                 0   -4.35300000    0.74100000   -1.48700000 H
H-H_                 0   -5.04600000    1.44900000    0.02500000 H

1 12 2.0 14 2.0
2 26 2.0 28 2.0
3 5 1.0 34 1.0
4 5 1.0 37 1.0
5 6 1.0 20 1.0
6 7 1.0 8 1.0 31 1.0
7
8 9 1.0 10 1.0 11 1.0
9
10
11 12 2.0 16 2.0
12 13 1.0
13
14 15 1.0 16 2.0
15
16 17 1.0
17 18 1.0 19 1.0 20 1.0
18
19
20 21 1.0 22 1.0
21
22 23 1.0 24 1.0 25 1.0
23
24
25 26 2.0 30 2.0
26 27 1.0
27
28 29 1.0 30 2.0
29
30 31 1.0
31 32 1.0 33 1.0
32
33
34 35 1.0 36 1.0 37 1.0
```

```
 34 35 1.0 36 1.0 37 1.0
 35
 36
 37 38 1.0 39 1.0
 38
 39
```

Step 3: Edit the `mm.type` file in the sictwo_files directory. Update the `mm.type` file with the following atom type conversions;

```
# Following format is required
# if($atom[$lnum] eq "UFF atom type") {$atomc[$lnum] = MMFF atom type};
#
if($atom[$lnum] eq "C_3") {$atomc[$lnum] = 1};
if($atom[$lnum] eq "C_R") {$atomc[$lnum] = 3 };
if($atom[$lnum] eq "H_") {$atomc[$lnum] = 23};
if($atom[$lnum] eq "S_R") {$atomc[$lnum] = 148 };
if($atom[$lnum] eq "O_3") {$atomc[$lnum] = 41 };
#
```

Step 4: Edit the `inp.par` file. Add the full path for the tinker `mmff.prm` file, which is located in the TINKER home directory. Apply the missing parameters as shown in the following `inp.par` file;

```
# ******************************************************
#     Path for the TINKER force field parameter file
# ******************************************************
parameters mmff
#
# ******************************************************
#         Define missing potential parameters
# ******************************************************
#
# Define atoms
#
# Define VWD parameters
#
# Define bond parameters
bond          73   73          520.00     1.3700
#
# Define bond angle parameters
angle         13   73   73       70.00     120.00
angle         74   73   73       70.00     111.00
#
# Define torsion parameters
torsion      74   16   74   73      0.000 0.0 1  10.750 180.0 2   0.000 0.0 3
torsion      74   16   74   39      0.000 0.0 1  10.750 180.0 2   0.000 0.0 3
torsion      13   73   73   74      0.000 0.0 1  10.750 180.0 2   0.000 0.0 3
torsion      13   73   73   13      0.000 0.0 1  10.750 180.0 2   0.000 0.0 3
torsion      74   73   73   74      0.000 0.0 1  10.750 180.0 2   0.000 0.0 3
#
```

Step 5: Copy Tinker executable files (`analysis, testgrad, testhess`) and the MMFF parameter file (`mmff.prm`) into the `sictwo_files` directory.

Step 6: Then, you can submit the calculations as a usual Gaussian09 job. Check the output files.

```
---------------------------- SICTWO Version 1.0 STARTED ----------------------------

MM calculations started
MM calculations finished ....
Information recovery

---------------------------- SICTWO Version 1.0 FINISHED ----------------------------
```

When the job is finished, total ONIOM(DFT:MMFF) energy can be found in the Gaussian09 output file.

```
 ONIOM: gridpoint  1 method:  low   system:  model energy:     0.061018663570
 ONIOM: gridpoint  2 method:  high  system:  model energy:  -976.426416941862
 ONIOM: gridpoint  3 method:  low   system:  real  energy:     0.077018098890
 ONIOM: extrapolated energy =    -976.410417506542
```

Ex2: Phenol system: ONIOM(B3LYP:OPLSAA) transition state optimization and frequency calculation. *(QM: Gaussian09 Rev.A02, MM:Tinker 7.1) version.*

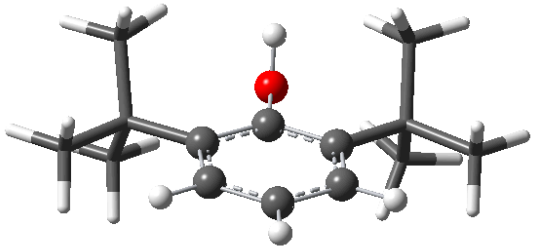

Figure 4. QM/MM molecular model of the phenol system ('ball and stick' model represents the QM region and 'tube' model represents the MM region).

Input file:

```
%nprocshared=8
%mem=8000MB
%chk=test
#p opt(ts,nomicro,calcfc,NoEigenTest,MaxCycle=150) freq oniom(b3lyp/6-
31G*:external="./sictwo_files/sictwo") geom=connectivity scf=maxcyc=100

ONIOM(B3LYP:OPLSAA) TS OPTn FREQ

0 1 0 1 0 1
 C-C_R             0    0.93462500   -0.09775200   -4.28614200 H
 C-C_R             0   -0.20004800   -0.46929100   -3.57830600 H
 C-C_R             0    2.06650000    0.31677900   -3.59139000 H
 H-H_R              0    2.96155200    0.61073300   -4.12152500 H
 C-C_R             0   -0.21498800   -0.43083300   -2.18468800 H
 C-C_R             0    2.04383400    0.35248300   -2.20027800 H
 H-H_R              0    2.93418700    0.67758400   -1.68416000 H
 C-C_R             0    0.91590800   -0.01547700   -1.45246100 H
 H-H_R              0    0.93081600   -0.13291200   -5.36680800 H
 C-C_3             0    0.92315500    0.03482700    0.07252400 L H-H_R 8
 C-C_A             0   -0.13262100    1.02833300    0.58472800 L
 H-H_            0    0.09595500    2.02901500    0.21849100 L
 H-H_            0   -1.15095500    0.80331200    0.27003700 L
 H-H_            0   -0.12116800    1.05053700    1.67538800 L
 C-C_A              0    0.69911700   -1.36831900    0.65992900 L
 H-H_            0    0.70127200   -1.31762500    1.74969300 L
 H-H_            0   -0.23394400   -1.83969600    0.35355900 L
 H-H_            0    1.50473500   -2.03149600    0.34542900 L
 C-C_A              0    2.26776300    0.51852000    0.61736500 L
 H-H_            0    2.22079700    0.53637700    1.70651700 L
 H-H_            0    3.08116000   -0.14593800    0.32797200 L
 H-H_            0    2.50083900    1.52633000    0.27553600 L
 O-O_R              0   -1.39856700   -0.82373600   -1.61623900 H
 H-H_A              0   -1.96380133   -0.05556463   -1.51444969 H
 C-C_A              0   -1.47926166   -0.93568810   -4.29781010 L H-H_R 2
 C-C_A              0   -1.82098471   -2.37151734   -3.85824241 L
 H-H_            0   -2.29076961   -2.34802965   -2.89717505 L
 H-H_            0   -2.48662201   -2.81351133   -4.56990828 L
 H-H_            0   -0.92299331   -2.95063225   -3.80223012 L
 C-C_A              0   -2.64425594    0.00350735   -3.93407912 L
 H-H_            0   -2.31531487    1.01987805   -3.99481108 L
 H-H_            0   -3.45341866   -0.15090397   -4.61695015 L
 H-H_            0   -2.97347804   -0.20589444   -2.93775402 L
 C-C_A              0   -1.25175743   -0.90545121   -5.82061264 L
 H-H_            0   -1.01351673    0.09201350   -6.12590841 L
 H-H_            0   -0.44285043   -1.55863895   -6.07342728 L
 H-H_            0   -2.14083413   -1.22871947   -6.32055290 L

 1 2 1.5 3 1.5 9 1.0
 2 5 1.5 25 1.0
 3 4 1.0 6 1.5
 4
 5 8 1.5 23 1.0
 6 7 1.0 8 1.5
 7
 8 10 1.0
 9
 10 11 1.0 15 1.0 19 1.0
 11 12 1.0 13 1.0 14 1.0
```

```
12
13
14
15 16 1.0 17 1.0 18 1.0
16
17
18
19 20 1.0 21 1.0 22 1.0
20
21
22
23 24 1.0
24
25 26 1.0 30 1.0 34 1.0
26 27 1.0 28 1.0 29 1.0
27
28
29
30 31 1.0 32 1.0 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37
```

mm.type file:

```
# Following format is required
# if($atom[$lnum] eq "G09_atom_type") {$atomc[$lnum] = MM3_atom_type};
#
if($atom[$lnum] eq "C_3") {$atomc[$lnum] = 84};
if($atom[$lnum] eq "C_A") {$atomc[$lnum] = 80};
if($atom[$lnum] eq "C_R") {$atomc[$lnum] = 90};
if($atom[$lnum] eq "H_") {$atomc[$lnum] = 85};
if($atom[$lnum] eq "H_R") {$atomc[$lnum] = 91};
if($atom[$lnum] eq "O_R") {$atomc[$lnum] = 109};
if($atom[$lnum] eq "H_A") {$atomc[$lnum] = 110};
#
#
```

inp.par file:

```
# ************************************************************
#     Path for the TINKER force field parameter file
# ************************************************************
#
parameters oplsaa
#
# ************************************************************
#         Define missing potential parameters
# ************************************************************
#
# Define atoms
#
# Define VWD parameters
#
# Define bond parameters
#
# Define bond angle parameters
#
# Define torsion parameters
#
```

ONIOM(DFT:MM3) energy of the optimized TS structure:

```
 ONIOM: gridpoint  1 method:  low   system:  model energy:      0.006197036209
 ONIOM: gridpoint  2 method:  high  system:  model energy:   -307.453843952164
 ONIOM: gridpoint  3 method:  low   system:  real  energy:     -0.009001773969
 ONIOM: extrapolated energy =    -307.469042762341
```

Ex3: Os complex: ONIOM(B3LYP:MM3) transition state optimization and frequency calculation. *(QM: Gaussian09 Rev.A02, MM:Tinker 7.1) version.*

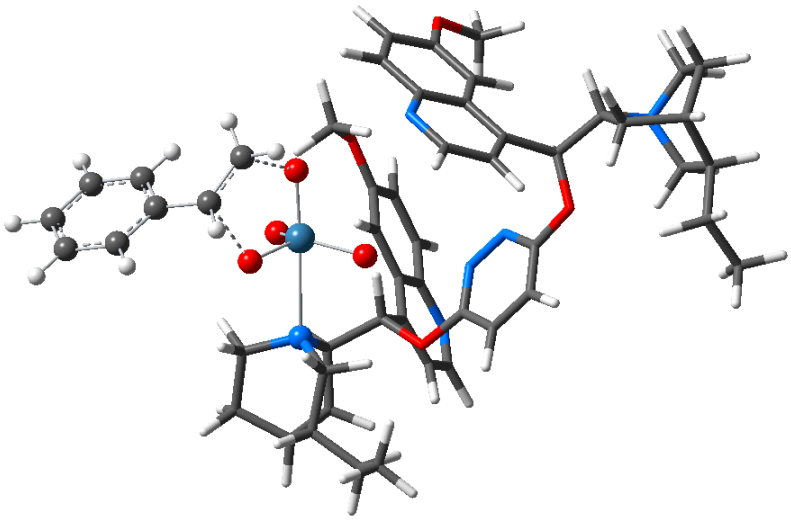

Figure 3. QM/MM molecular model of Os complex ('ball and stick' model represents the QM region and 'tube' model represents the MM region).

Input file:

```
%nprocshared=8
%mem=8000MB
%chk=test
#p opt(ts,calcfc,nomicro,noeigentest) freq
oniom(b3lyp/genecp:external="./sictwo_files/sictwo") geom=connectivity

ONIOM(B3LYP:MM3) TS OPT FREQ

0 1 0 1 0 1
 Os-X             0   -2.33776600   -0.83263200   -0.44889700 H
 O-O_3            0   -0.94768600   -0.16030500   -1.22534700 H
 O-O_3            0   -3.63674500   -1.23514900   -1.57651000 H
 O-O_3            0   -1.84473800   -2.51073000   -0.21824800 H
 O-O_3            0   -2.89900300   -0.40944900    1.13020900 H
 N-N_3            0   -3.17669100    1.57198900   -0.79789900 H
 C-C_R            0   -4.05204500   -3.27377600   -1.86204100 H
 C-C_R            0   -2.91848100   -3.90196700   -1.36782800 H
 H-H_             0   -2.05923800   -4.05356500   -2.01011800 H
 H-H_             0   -4.06570800   -3.00882600   -2.91410300 H
 C-C_3          0   -2.70107200    2.56876300    0.19381900 L H-H_ 6   0.0000
 C-C_3          0   -2.86627900    1.97333500   -2.17754500 L H-H_ 6   0.0000
 C-C_3          0   -4.64193900    1.47024300   -0.67223500 L H-H_ 6   0.0000
 O-O_R            0   -0.55334600   -0.37679800    4.80953000 L
 O-O_R            0   -0.43724800    2.96979900   -0.62351400 L
 C-C_R            0   -0.79624900    3.28698600    1.73974500 L
 C-C_R            0   -0.57187800    4.60378900    1.60102900 L
 C-C_R            0   -0.20195800    5.34359000    2.64741100 L
 C-C_R            0   -0.19580500    3.59309000    3.97375700 L
 C-C_R            0    0.03075100    3.09604600    5.19743600 L
 C-C_R            0   -0.10003600    1.78980100    5.44524300 L
 C-C_R            0   -0.47252300    0.94715500    4.47249900 L
 C-C_R            0   -0.70946400    1.44843300    3.24525500 L
 C-C_R            0   -0.57863900    2.76486700    2.97095600 L
 C-C_3            0   -0.80010400   -1.34787400    3.79099800 L
 N-N_R            0   -0.02164000    4.85325900    3.81233000 L
 C-C_3            0   -1.19053800    2.47210500    0.49466400 L
 C-C_3            0   -3.17099400    3.97353700   -0.25667500 L
 C-C_3            0   -4.26338200    3.84572400   -1.32832400 L
 C-C_3            0   -5.31051700    2.85544200   -0.80098700 L
 N-N_R            0    1.30633600    1.75245200    0.19710800 L
 C-C_3            0   -3.65129700    3.23782500   -2.60607100 L
 C-C_3            0   -2.77863500    4.22879800   -3.39870000 L
 C-C_3            0   -2.31566900    3.67155900   -4.75238100 L
 C-C_R            0    0.80068200    2.41902200   -0.77546900 L
 C-C_R            0    1.40841600    2.50704500   -1.95886400 L
 N-N_R            0    1.32247800   -3.44258700   -1.30724700 L
 N-N_3            0    6.74372100   -0.38115100    0.27073600 L
 N-N_R            0    2.41428700    1.15488200    0.05916100 L
 O-O_R            0    2.51714900   -3.08141900    3.89747400 L
 O-O_R            0    4.19232900    0.48353100   -1.19380400 L
 C-C_R            0    3.25544000   -1.67724700   -0.60804300 L
 C-C_R            0    2.85417800   -1.83390800   -1.87985100 L
 C-C_R            0    1.90152100   -2.71711100   -2.18462100 L
 C-C_R            0    1.67317000   -3.30785500   -0.08096100 L
 C-C_R            0    1.04458900   -4.06796600    0.82630400 L
 C-C_R            0    1.34487900   -3.97889800    2.12547400 L
 C-C_R            0    2.29246800   -3.13077800    2.54855300 L
 C-C_R            0    2.92138700   -2.36496100    1.63753500 L
```

```
C-C_R             0    2.63109500   -2.43797000    0.32087500 L
C-C_3             0    3.32078300   -2.02643100    4.43100700 L
C-C_3             0    4.31941300   -0.61436900   -0.27805600 L
C-C_3             0    7.93766200   -1.19216200    0.52646700 L
C-C_3             0    8.45169400   -1.82123600   -0.78790600 L
C-C_3             0    7.69055400   -1.18246500   -1.96218400 L
C-C_3             0    6.20561500   -1.55488400   -1.81412100 L
C-C_3             0    5.72870500   -1.22664100   -0.38052500 L
C-C_3             0    7.13249600    0.77879200   -0.53660700 L
C-C_3             0    7.85061300    0.34761900   -1.84061600 L
C-C_3             0    7.34303000    1.11511500   -3.07553600 L
C-C_3             0    7.67965100    2.61242800   -3.03235800 L
C-C_R             0    3.04816900    1.21175900   -1.05450200 L
C-C_R             0    2.57171100    1.88350100   -2.10290900 L
H-H_              0   -0.68649000    5.09883800    0.62362700 L
H-H_              0   -0.03392000    6.42694300    2.51965700 L
H-H_              0    0.34435700    3.77307100    6.01077400 L
H-H_              0    0.10815000    1.40286100    6.45768000 L
H-H_              0   -1.00794100    0.75195500    2.45192100 L
H-H_              0   -0.73466900   -2.36189200    4.23534100 L
H-H_              0   -1.81979000   -1.22651100    3.37332300 L
H-H_              0   -0.04317000   -1.27908800    2.98265300 L
H-H_              0   -0.96378300    1.40007800    0.64698200 L
H-H_              0   -3.21465200    2.33715200    1.15712700 L
H-H_              0   -2.33147300    4.56899500   -0.66964300 L
H-H_              0   -3.55602000    4.54270100    0.61986600 L
H-H_              0   -4.73131100    4.83487400   -1.54113300 L
H-H_              0   -6.18709400    2.80303200   -1.48548700 L
H-H_              0   -5.69362800    3.19757700    0.18714900 L
H-H_              0   -4.91517200    1.00826200    0.30171800 L
H-H_              0   -5.04281000    0.79168200   -1.45655300 L
H-H_              0   -3.11034100    1.13786700   -2.87058400 L
H-H_              0   -1.77670100    2.13616500   -2.28862500 L
H-H_              0   -4.49443600    2.92850300   -3.27044100 L
H-H_              0   -1.88531000    4.52241300   -2.80331400 L
H-H_              0   -3.35898500    5.16348200   -3.57774600 L
H-H_              0   -1.71592100    4.42220900   -5.31448400 L
H-H_              0   -1.67933700    2.76690500   -4.63428400 L
H-H_              0   -3.17903300    3.39066100   -5.39588000 L
H-H_              0    0.94678700    3.05245300   -2.79828300 L
H-H_              0    3.30090700   -1.23850500   -2.69269300 L
H-H_              0    1.58432300   -2.83864500   -3.23474100 L
H-H_              0    0.26155000   -4.77307100    0.49787000 L
H-H_              0    0.80447800   -4.60682500    2.85467100 L
H-H_              0    3.69391200   -1.66760900    1.98895400 L
H-H_              0    3.32528400   -2.10095800    5.53759200 L
H-H_              0    4.37021300   -2.11142000    4.08086700 L
H-H_              0    2.90401700   -1.03454600    4.15753000 L
H-H_              0    4.19480700   -0.23556600    0.75744300 L
H-H_              0    7.70672400   -1.98681300    1.27015500 L
H-H_              0    8.72855700   -0.56052900    0.98848500 L
H-H_              0    8.28666600   -2.92259400   -0.78255200 L
H-H_              0    9.54831700   -1.66036200   -0.89338300 L
H-H_              0    8.09574100   -1.54799800   -2.93437200 L
H-H_              0    6.05856400   -2.63916900   -2.02183800 L
H-H_              0    5.60842100   -1.01206300   -2.57558000 L
H-H_              0    5.69034600   -2.18383900    0.19169800 L
H-H_              0    7.80528300    1.43473100    0.05968000 L
```

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H-H_              0    6.24258600    1.40031500   -0.75796700 L
H-H_              0    8.94138100    0.56526500   -1.73653700 L
H-H_              0    6.24196100    0.99417800   -3.18281100 L
H-H_              0    7.79913700    0.67405900   -3.99202500 L
H-H_              0    7.32640600    3.13257700   -3.95096100 L
H-H_              0    7.20395600    3.12100400   -2.16506400 L
H-H_              0    8.77686900    2.78293300   -2.95846100 L
H-H_              0    3.10856800    1.89497700   -3.06561400 L
H-H_              0   -2.95997400   -4.51727900   -0.47808800 H
C-C_R             0   -5.36070500   -3.29923600   -1.19268000 H
C-C_R             0   -6.52726200   -3.10396300   -1.95158600 H
C-C_R             0   -5.48834900   -3.49960300    0.19444900 H
C-C_R             0   -7.78478300   -3.13040600   -1.35120200 H
H-H_              0   -6.44138700   -2.93686400   -3.02272700 H
C-C_R             0   -6.74487100   -3.52034500    0.79446000 H
H-H_              0   -4.59916000   -3.61857900    0.80695000 H
C-C_R             0   -7.89821800   -3.34056600    0.02474500 H
H-H_              0   -8.67560800   -2.98553000   -1.95659500 H
H-H_              0   -6.82491100   -3.67135600    1.86758700 H
H-H_              0   -8.87710400   -3.35894300    0.49610100 H

1 2 1.0 3 1.0 4 1.0 5 1.0
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6 11 1.0 12 1.0 13 1.0
7 8 1.5 10 1.0 117 1.0
8 9 1.0 116 1.0
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11 27 1.0 28 1.0 73 1.0
12 32 1.0 81 1.0 82 1.0
13 30 1.0 79 1.0 80 1.0
14 22 1.0 25 1.0
15 27 1.0 35 1.0
16 17 2.0 24 2.0 27 1.0
17 18 2.0 64 1.0
18 26 2.0 65 1.0
19 20 2.0 24 2.0 26 2.0
20 21 2.0 66 1.0
21 22 2.0 67 1.0
22 23 2.0
23 24 2.0 68 1.0
24
25 69 1.0 70 1.0 71 1.0
26
27 72 1.0
28 29 1.0 74 1.0 75 1.0
29 30 1.0 32 1.0 76 1.0
30 77 1.0 78 1.0
31 35 2.0 39 1.5
32 33 1.0 83 1.0
33 34 1.0 84 1.0 85 1.0
34 86 1.0 87 1.0 88 1.0
35 36 2.0
36 63 2.0 89 1.0
37 44 2.0 45 2.0
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38 53 1.0 57 1.0 58 1.0
 39 62 2.0
 40 48 1.0 51 1.0
 41 52 1.0 62 1.0
 42 43 2.0 50 2.0 52 1.0
 43 44 2.0 90 1.0
 44 91 1.0
 45 46 2.0 50 2.0
 46 47 2.0 92 1.0
 47 48 2.0 93 1.0
 48 49 2.0
 49 50 2.0 94 1.0
 50
 51 95 1.0 96 1.0 97 1.0
 52 57 1.0 98 1.0
 53 54 1.0 99 1.0 100 1.0
 54 55 1.0 101 1.0 102 1.0
 55 56 1.0 59 1.0 103 1.0
 56 57 1.0 104 1.0 105 1.0
 57 106 1.0
 58 59 1.0 107 1.0 108 1.0
 59 60 1.0 109 1.0
 60 61 1.0 110 1.0 111 1.0
 61 112 1.0 113 1.0 114 1.0
 62 63 2.0
 63 115 1.0
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 117 118 1.5 119 1.5
 118 120 1.5 121 1.0
 119 122 1.5 123 1.0
 120 124 1.5 125 1.0
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 122 124 1.5 126 1.0
 123
 124 127 1.0
 125
 126
 127

Os 0
LanL2DZ
****
O 0
6-31G*
****
C H N 0
6-31G
****

Os 0
LanL2DZ
```

mm.type file

```
# Following format is required
# if($atom[$lnum] eq "G09_atom_type") {$atomc[$lnum] = MM3_atom_type};
#
   if($atom[$lnum] eq "X")  {$atomc[$lnum] = 165};
   if($atom[$lnum] eq "C_3") {$atomc[$lnum] = 1};
   if($atom[$lnum] eq "H_")  {$atomc[$lnum] = 5};
   if($atom[$lnum] eq "O_3") {$atomc[$lnum] = 7};
   if($atom[$lnum] eq "O_R") {$atomc[$lnum] = 6};
   if($atom[$lnum] eq "C_R") {$atomc[$lnum] = 2};
   if($atom[$lnum] eq "N_3") {$atomc[$lnum] = 8};
   if($atom[$lnum] eq "N_R") {$atomc[$lnum] = 37};
#
```

inp.par file:

```
parameters mm3
#
# *****************************************************
#         Define missing potential parameters
# *****************************************************
#
# Define atoms
atom      165      X        "Os system"   76        190.23      4
# Define VWD parameters
vwd       165      0.037    1.560
# Define bond parameters
bond      7        165      0.3           1.67
bond      8        5        6.420         1.0150
# Define bond angle parameters
angle     7        165      7             0.5       90.0
angle     6        2        37            0.6       120.0
angle     5        8        5             0.605     106.40
# Define torsion parameters
torsion   2   1    6    2         0.0  0.0 1    0.0 180.0 2     0.403 0.0 3
torsion   6   2    37   37        0.0  0.0 1   12.0 180.0 2     0.0   0.0 3
torsion   1   6    2    37        1.05 0.0 1    7.5 180.0 2    -0.2   0.0 3
```

ONIOM(DFT:MM3) energy of the optimized transition state:

```
 ONIOM: gridpoint  1 method:  low   system:  model energy:     0.124938477760
 ONIOM: gridpoint  2 method:  high  system:  model energy:  -758.044727877941
 ONIOM: gridpoint  3 method:  low   system:  real  energy:     0.325921682919
 ONIOM: extrapolated energy =    -757.843744672782
```