# User Manual

For executing the TORQUE program, users need to install a fortran compiler such as the intel fortran compiler or gfortran. In this manual we explain how to install gfortran on a linux machine. Based on the distribution of the linux, gfortran can be install either one of this method.

Debian base linux distributions such as ubuntu:

sudo apt-get install gfortran

Fedora:

su yum install gfortran

the last version of TORQUE program can be downloaded from this address: *https://github.com/ayatghazi/Torque-Method*. After downloading the zip file, users can extract it by this command:

tar -xzvf TORQUE.1.0.2

For compiling the program users can follow these command:

Make TQ0

Make

The executable file will generate by these commands and can be execute by:

./TQ

Please note that users must provide an input file for desirable structure with a format which will be explained in continue. However, we have prepared some example input files. Users can copy them from Example_inputfile folder to the main folder of the program, and rename the file to inputfile.

Furthermore, we provide a detailed description of the input file for the TORQUE program setup of Grimselite as an example in this manual. The input file consists of different sections which are delimited by a beginning and an ending line. Any line which starts with (‘#’, ‘!’, ‘c’) is considered as a comment by the program.

Grimselite crystal has hexagonal lattice with 44 atoms inside the unit cell. The X-ray diffraction data for lattice parameters and atomic positions are (Li & Burns, 2001):

a=9.3020 b=9.3020 c=8.2600 α=90.0 β=90.0 γ=120.0

Space Group=" P" "6"¯"2c"

| atom | x | y | z | occupancy |
|---|---|---|---|---|
| U | 0.6667 | 0.3333 | 0.7500 | 1.0 |
| K | 0.2921 | 0.0000 | 0.0000 | 1.0 |
| Na | 0.3333 | 0.6667 | 0.7500 | 1.0 |
| O1 | 0.9694 | 0.4797 | 0.7500 | 1.0 |

| | | | | |
|---|---|---|---|---|
| O2 | 0.8485 | 0.6315 | 0.7500 | 1.0 |
| O3 | 0.6667 | 0.3333 | 0.9673 | 1.0 |
| O4 | 0.1274 | 0.757 | 0.7500 | 1.0 |
| O5 | 0.0000 | 0.0000 | 0.1277 | 0.5 |
| C | 0.9883 | 0.6282 | 0.7500 | 1.0 |

The input file starts with information about the lattice:

```
LATTICE_MATRIX_
   9.3020      0.0000      0.0000
  -4.6510      8.0558      0.0000
   0.0000      0.0000      8.2600
END_LATTICE_MATRIX_
```

The second section defines atomic species (second column) with their associated oxidation state (third column). First column is an identifier integer number (IN1) which distinguish different atomic species or the same atomic species with different symmetries. Charges for the oxygen and hydrogen atoms of crystallization water can be set, but the program will reset value to the selected water model. Framework oxygen is treated as any other ion in the structure and has the same syntax. Note that program reads the charges as real values, so users are not limited to integer oxidation numbers:

```
ATOMIC_SPECIES_CHARGES_
 1    U     6.0
 2    K     1.0
 3    Na    1.0
 4    O    -2.0
 5    O    -2.0
 6    O    -2.0
 7    O    -2.0
 8    O    -2.0
 9    C     4.0
END_ATOMIC_SPECIES_CHARGES_
```

The next section lists atomic positions and their occupancy numbers. Each line begins with a integer number (IN1), and follows by a position coordination and an occupation number. IN1 is the identifier number which was defined in previous section. Positions that belong to the same crystallographically

equivalent set have the same integer number. In the case of partial occupancy, users can exclude atoms in this section by deletion or inserting comment lines. Alternatively, average structures can be specified through occupation numbers for each site. If a position randomly occupied by several different atom species, its coordination must be repeated in the following section with different IN1s and corresponding occupation numbers to have a proper average structure.

ATOMIC_POSITIONS_OCCUPANCY_

| | | | | |
|---|---|---|---|---|
| 1 | 0.66670 | 0.33330 | 0.75000 | 1.0 |
| 1 | 0.33330 | 0.66670 | 0.25000 | 1.0 |
| 2 | 0.29210 | 0.00000 | 0.00000 | 1.0 |
| 2 | 0.00000 | 0.29210 | 0.00000 | 1.0 |
| 2 | 0.70790 | 0.70790 | 0.00000 | 1.0 |
| 2 | 0.29210 | 0.00000 | 0.50000 | 1.0 |
| 2 | 0.00000 | 0.29210 | 0.50000 | 1.0 |
| 2 | 0.70790 | 0.70790 | 0.50000 | 1.0 |

…

# lines with IN1=8 show the coordinates of oxygen atoms of water molecule with half occupancy.

| | | | | |
|---|---|---|---|---|
| 8 | 0.00000 | 0.00000 | 0.12770 | 0.5 |
| 8 | 0.00000 | 0.00000 | 0.37230 | 0.5 |
| 8 | 0.00000 | 0.00000 | 0.62770 | 0.5 |
| 8 | 0.00000 | 0.00000 | 0.87230 | 0.5 |

# Following lines are the positions of hydrogen atoms which have found by DFT computations.

| | | | | |
|---|---|---|---|---|
| 10 | 0.016663 | -0.078797 | 0.193012 | 1.0 |
| 11 | -0.078894 | 0.017694 | 0.191793 | 1.0 |
| 12 | -0.078797 | 0.016663 | 0.693012 | 1.0 |
| 13 | 0.017694 | -0.078894 | 0.691793 | 1.0 |

END_ATOMIC_POSITIONS_OCCUPANCY_

In Grimselite water is located in crystallographic site 4e site with 50% occupancy (2 oxygen and 4 hydrogen ions). The oxygen atoms of water molecules have index IN1=8. As it can be seen, the occupation numbers for these oxygen atoms are 0.5 in column 5. In this case, the program deals with random average occupations of the crystallographically equivalent positions. Alternatively, users can specify the two water locations explicitly and changing the occupation number for oxygen atoms to 1.

The oxygen atoms that belong to water molecules must be identified with their IN1 number in the following section:

WATER_IDENTIFICATION_NUMBER_

8

END WATER_IDENTIFICATION_NUMBER_

In the next section, the user must indicate the IN1 numbers of hydrogen atoms of water molecules. The program does not consider those atom species which their IN1 number are listed here in the calculation of electrostatic forces. Here, the hydrogen atoms with IN1=10 to 13 are completing the description of the water molecule, and must be specified. If there is no information about the coordinates of hydrogen atoms of water molecules, this section could be blank or zero:

HYDROGEN_IDENTIFICATION_NUMBER_

10 11 12 13

END HYDROGEN_IDENTIFICATION_NUMBER_

The type of water models is defined in the next section. 0 = TIP3P, 1 = TIP4P/2005, 2 = TIP5P. Default is TIP3P.

WATER_MODEL_

0

END_WATER_MODEL_

We have defined some default parameters for the minimum torque magnitude, maximum and minimum degree of angular rotation, and a seed value which is used to initialize the random number generator for assigning random orientations to water molecules. Their default values are listed below. Users can change these values, and the new values will be overwritten:

PARAMETERS_

Threshold = 0.00005

Max_Angle = 0.5

Min_Angle = 0.005

Seed = 12345

END_PARAMETERS_

The symmetry operations are listed in this last section of the input files. These operators are combination of rotations/translations {R|t} and stored in a 2d array (sym). Each set of rotation/translation consists of three successive lines which labeled by the same number in the first column. Columns two to four are showing the components of the rotation matrix (by row), and the fifth column shows the non-symmorphic translation vector. For instance, there are three lines which are started with number 1 in the first column.

These three lines indicate an operator consist of a 3×3 rotation matrix and a 3×1 translation vector. As it can be seen here, the first line starts with number zero at the first column. Lines starting with zero in the first column are used to specify the origin of the space group as well as centering (P, F, I, C, A, R,…). "P" requires only one centering vector (0,0,0), so there is one line that starts with zero at the beginning as shown in the example. A "F" lattice in the conventional basis requires 4 lines in the block with zero in the first column to keep the coordination of the origin and possible centering vector(s), (0,0,0), (1/2,1/2,0), (1/2,0,1/2), (0,1/2,1/2) on each line in the columns two to four (fifth column is zero as well).

```
SYMMETRY_OPERATORS_
 0     0.00000     0.00000     0.00000     0.00000
 1     1.00000     0.00000     0.00000     0.00000
 1     0.00000     1.00000     0.00000     0.00000
 1     0.00000     0.00000     1.00000     0.00000
…
12    -1.00000     0.00000     0.00000     0.00000
12    -1.00000     1.00000     0.00000     0.00000
12     0.00000     0.00000     1.00000     0.50000
END_SYMMETRY_OPERATORS_
```

For a face-centered, "F" lattice, the first four lines read as follows:

```
 0    0.00000    0.00000    0.00000    0.00000
 0    0.50000    0.50000    0.00000    0.00000
 0    0.50000    0.00000    0.50000    0.00000
 0    0.00000    0.50000    0.50000    0.00000
```

This completes the description of the input file for TORQUE. A detailed listing of this file and other examples are available in the source code distribution.