

Force Field Fitting Toolkit

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Force field fitting toolkit consists of four independent codes allowing fitting of the following parameters:

1. Fitting partial charges and atomic polarizabilities in order to represent electrostatic potential around a molecule and molecular polarizability obtained from *ab initio* quantum chemistry calculations.
2. Fitting parameters for torsional, bending and bonding potentials.
3. Fitting parameters for nonbonded part of the force fields (without geometry optimization).
4. Fitting parameters for nonbonded part of the force fields (including geometry optimization).

Below we briefly describe the forms of force fields, which could be developed using this toolkit, followed by description of each of four toolkits.

Classical Force Field

In the classical force field employed here, the total potential energy of the ensemble of atoms, represented by the coordinate vector \mathbf{r} , is denoted as $U^{\text{tot}}(\mathbf{r})$. The latter is represented as a sum of nonbonded interactions $U^{\text{NB}}(r_{ij})$ as well as energy contributions due to the distortion of bonds $U^{\text{BOND}}(r_{ij})$, bends $U^{\text{BEND}}(\theta_{ijk})$ and torsions $U^{\text{TORS}}(\phi_{ijkl})$ and is given by

$$U^{\text{tot}}(\mathbf{r}) = \sum_{i < j} U^{\text{NB}}(r_{ij}) + \sum_{ij} U^{\text{BOND}}(r_{ij}) + \sum_{ij k} U^{\text{BEND}}(\theta_{ijk}) + \sum_{ij k l} U^{\text{TORS}}(\phi_{ijkl}) \quad (1)$$

The nonbonded energy $U^{\text{NB}}(r_{ij})$ (eq.2) consists of the sum of two-body repulsion and dispersion energy terms $U^{\text{R/D}}(r_{ij})$ modeled by Lennard–Jones (eq.3) or Buckingham potentials (eq.4) plus electrostatic, and polarization $U^{\text{POL}}(r_{ij})$ energies:

$$U^{\text{NB}}(r_{ij}) = U^{\text{R/D}}(r_{ij}) + \frac{332.07q_i q_j}{r_{ij}} + U^{\text{POL}}(r_{ij}) \quad (2)$$

$$U^{\text{R/D}}(r_{ij}) = A_{ij} \exp(-B_{ij} r_{ij}) - C_{ij}/r_{ij}^6 \quad (3)$$

$$U^{\text{R/D}}(r_{ij}) = A'_{ij} / r_{ij}^{12} - C_{ij}/r_{ij}^6 \quad (4)$$

where q_i , q_j are partial charges of atoms i and j , r_{ij} is the atomic separation in Å, A_{ij} , B_{ij} and A'_{ij} are the repulsion parameters and C_{ij} is the dispersion parameter.

The potential energy due to dipole polarization is not pair-wise additive and is given by

$$U^{\text{pol}} = - \sum_i \boldsymbol{\mu}_i \cdot \mathbf{E}_i^0 + 0.5 \sum_i \sum_j \boldsymbol{\mu}_i \cdot \mathbf{T}_{ij} \cdot \boldsymbol{\mu}_j + U^{\text{self}} \quad (5)$$

where \mathbf{E}_i^0 is the electric field at atom i generated by the permanent charges in the system, $\boldsymbol{\mu}_i$ is the induced dipole moment at atom i , \mathbf{T}_{ij} is the second order dipole tensor, U^{self} is the energy required to induce the dipole moments $\boldsymbol{\mu}_i$, $\boldsymbol{\mu}_j = \alpha_i \mathbf{E}_{\text{tot}}$, where α_i is the isotropic atomic polarizability, and \mathbf{E}_{tot} is the total electrostatic field at the atomic site i due to permanent charges and induced dipoles.

Contributions from bond stretching $U^{\text{BOND}}(r_{ij})$ and angle bending $U^{\text{BEND}}(\theta_{ijk})$ are included in the potential as using the following relations:

$$U^{\text{BOND}}(r_{ij}) = \frac{1}{2} k^{\text{BOND}} (r_{ij} - r_{ij}^0)^2 \quad (6)$$

$$U^{\text{BEND}}(\theta_{ijk}) = \frac{1}{2} k^{\text{BEND}} (\theta_{ijk} - \theta_{ijk}^0)^2 \quad (7)$$

where r_{ij}^0 is the equilibrium bond length between atoms i and j , θ_{ijk}^0 is the equilibrium angle between atoms i , j and k .

Finally, torsional potential is given by eq. 8

$$U^{\text{TORS}}(\phi_{ijkl}) = \frac{1}{2} \sum_n k_{ijkl}^T \cos(n \phi_{ijkl}) \quad (8)$$

where k_{ijkl}^T is a torsional energy parameters, ϕ_{ijkl} is a torsional angle.

Code for Fitting Partial Charges and Atomic Polarizabilities (“qfit.f”)

Partial charges and atomic polarizabilities could be determined fitting the electrostatic potential and molecular polarizability obtained from *ab initio* quantum chemistry calculations.

Input parameters for this code are:

- a file containing electrostatic potential on a grid of points around a molecule, which could be obtained using *cube* keyword in Gaussian 98 quantum chemistry package. A number of such files can be used in a fit of one set of partial charges.
- “qfit.inp” is file specifying the dipole moment and molecular polarizability of a molecule as well as information about additional constrains such as a total charge of oligomers repeat unit being zero, etc.
- “qfit.f” is the fitting program
- “qfit.par” is the parameter file containing information about maximum number of atoms in a molecule, number of charge types, etc.
- “h.inp” is a file specifying initial interval for differentiation
- “oopt.par” parameters for the minimizer

We illustrate fitting partial charges and polarizability for PEO model based upon *ab initio* quantum chemistry data for 1,2-dimethoxyethane and dimethyl ether. Electrostatic grid was generated using *cube=(22,potential)* keyword in Gaussian98 code for two DME ($\text{CH}_3\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_3$) conformers trans-trans-trans, trans-gauche-trans and for a complex containing two dimethyl ether molecules. The files containing electrostatic grids were named *cube_ttt*, *cube_tgt*, and *cube_2ethers*, respectively. At the next step “qfit.inp” file is created according to the following rules:

File “qfit.inp”

Line1: You have two options .TRUE. or .FALSE. If one wants to fit parameters .TRUE. should be input in the Line1. However, if one only desires to check how a given set of parameters describes the electrostatic grid, molecular dipole moment and molecular polarizability without fitting parameters, .FALSE. should be used.

Line 2: Input .TRUE. for fitting polarizable potential and .FALSE. otherwise.

Line 3: If one fits polarizable potential, then two options are available. Option (a) is to exclude charge-(induced dipole) and (induced dipole)-(induced dipole) interactions between atoms from interaction list only for bonded atoms (1-2 interaction, one should input 2 in the second line) and option (b) is to exclude charge-(induced dipole) and (induced dipole)-(induced dipole) interactions between atoms from interaction list for atoms connected by bonds and bends (1-2-3 interactions, one should input 3 in the second line). Description of bonds and bends should be given in the files with names *bondsN.inp*, where *N* is the number of the complex. In our example, files “bonds1.inp”, “bonds2.inp” and “bonds3.inp” contain information about bonds and bends.

Line 4: Input a number of complexes in the fit

Line 5: Input the name of the file containing electrostatic grid for the first geometry

Line 6: Weight given to the first geometry in the fit

Line 7: Enter components of the dipole moment for the first complex (in Debye)

Line 8: Enter molecular polarizability tensor in (\AA^3) in the order α_{xx} , α_{yx} , α_{yy} , α_{xz} , α_{yz} , α_{zz} .

Line 9: Comment line

Line 10: Input a list of charge types for each type for the first complex

Line 11: Comment line

Line 12: Input a number of additional constrains. Description of each constrain will take two lines. Additional constrains might constitute constraining a charge of ions to 1,2, etc. or constraining a charge of repeat units to zero. In the case of DME, we constrain charges of repeat units to zero, in order to be able to extrapolate the developed force field to PEO. Additional constrains are implemented by means of addition

of a penalty function: $w \left(\sum_j^{N_c} q_j - q_c \right)$, where w is the weight of the penalty function, N_c is the number of

atoms in the charge groups (monomer, charge group), q_c is the desired charge of the charge group.

Line 13: Input w N_c q_c (separated by spaces)

Line 14: Input q_j (atoms constituting constrained charge group)

Lines 15-16,17-18,19-20 include description of additional constrains for another charge groups

Lines 21-49 describe complex 2-3 corresponding to cube_tgt and cube_2ether files with electrostatic grids

Line 49: Comment line

Lines 50-53: Input q_i , α_i , $weight_i$, where q_i is the initial charge for charge-type i , α_i is the initial atomic polarizability value for type i . It is possible to constrain atomic polarizability to a certain value. In order to do that a big number should be input as $weight_i$, zero should be input otherwise. Line51 has parameters for the first atom-type, Line52 has parameters for the second atom-type, etc.

Line 54: comment line

Line 55: weight for fitting partial charges and atomic polarizabilities to yield electrostatic grid from quantum chemistry calculations

Line 56: weight for constraining molecular dipole moment from force field to that from quantum chemistry (line 7, etc)

Line 57: weight for fitting atomic polarizabilities to yield given molecular polarizabilities

File "qfit.par"

parameter (maxat = 18)	! maximum number of atoms in each complex
parameter (maxbonds=16)	! maximum number of bonds
parameter (maxbends=26)	! maximum number bends
parameter (maxcharges=4)	! exact number of charges
parameter (maxgeom=3)	! maximum number of geometries
parameter (maxnum = 40)	! maximum number grids in each direction
parameter (maddconstr=10)	! maximum number of additional constrains
parameter (head=3.5d0)	! the cutoff for inclusion of electrostatic grid points in the calculation

Only electrostatic grid points closer than "head" to any atom are included in the calculations, while electrostatic grid points closer than Van der Waals radii are excluded from the analysis. Van der Waals radii are given in *vdr* array in *qfit.f* program. The default values are 1.5 Å for H, 2.0 Å for the other atoms.

The Broyden-Fletcher-Goldfarb-Shanno variant of Davidson-Fletcher-Powell minimization algorithm was implemented. Parameters for this minimizer are given in the "oopt.par" file. The starting Δ for calculation of numerical derivatives is given in "h.inp" file for each parameter if .FALSE. is input in the first line. If .TRUE. is in the first line than the parameter Δ from the second line is used for all parameters.

Code for Fitting Torsional, Bonding and Bending Potentials

Accurate representation of relative populations of polymer conformations is important for correct representation of local and global polymer static properties, while accurate description of barriers for conformational transitions is vital for quantitative prediction of polymer dynamics. The code "tfit.f" is designed for fitting torsional (eq. 8), bending (eq. 7) and bonding (eq.6) potentials responsible for the prediction of the above properties. Usually, the torsional energy parameters (k_{ijkl}^T) (eq. 8) are determined in order to give the best description of relative conformational energies, conformer geometries and barriers for conformational transitions, which could be determined from *ab initio* quantum chemistry calculations. The equilibrium bond length between atoms i and j (r_{ij}^0) (eq. 6) and the equilibrium angle between atoms i , j and k (θ_{ijk}^0) (eq. 7) are determined by fitting conformer geometries. Although "tfit.f" code was designed to fit torsional (eq. 8), bending (eq. 7) and bonding (eq.6) potentials, it also allows fitting nonbonded parameters (eq. 3-4) and atomic polarizabilities based upon intermolecular complex energies.

In order to perform fitting with "tfit.f" code, one need the following files

- “tfit.f” is the main program.
- “tfit.inp” is the file containing relative conformational energies, parameters for conformer drive as well as various fitting options.
- “geoms.inp” is the file, containing conformer geometries in XMOL-XYZ format.
- “params.h”, “dimensions.h”, “commons.h” are the files containing array dimensions, array description, optimizer options, and a list of common variables used by the program. Only “params.h” file should be modified.
- “fort.11” is the file, containing information about bond, bend and torsion assignment. For example, how many bonds are in each chain, how many chains are in the system, which atoms are connected by a specific bonds, bends and torsions, etc.
- “fort.26” is the file, specifying initial coordinates for each atom and atom-types for each atom
- “fort.25” is not extensively used by “tfit.f” program, but should be present. Only cutoff radius and box size are read from this file.

We will explain how to use “tfit.f” program for fitting fitting torsional, bending and bonding potentials using a simple butane molecule as an example.

File “tfit.inp”

```
.false.      ! .TRUE.-fit parameters, .FALSE.-do not fit parameters
.TRUE.      ! .TRUE.-optimize geometries, .FALSE.-use geometries as given
.TRUE.      ! .TRUE.-compute analytical derivatives,.FALSE.-numerical deriv.
.false.     ! read the geometries from "geoms.inp"
.false.     ! subtract energy of the first geometry from all the other
1           ! in the torsional fit this geometry has a zero energy (1st geom)
0.000      ! Energy to add to all complex energies
5          ! number of complexes(geometries) in the fit
Line1.Energy,weight_energy,w-zero-force;Line2.Number of bonds,bends,torsions,artificial bonds to constrain and Line3.weights
# fi=180.0 (comment line)
0.000 0.0 0.000 (conformer energy, weight for conformer energy, weight for constraining force to zero)
0 0 1 0 1000.0 1000.0 10.0 1000.00 (Number of bonds,bends,torsions,artificial bonds to constrain)
10 180.0      (constrain torsion number 10 (see fort.11) to 180 degrees)
# fi=150.0 constrained (comment line)
0.000 00.0 0.000
0 0 1 0 1000.0 1000.0 10.0 1000.00
10 150.0     (constrain torsion number 10 (see fort.11) to 150 degrees)
# fi=120 constrained (comment line)
3.0 1.0 1.000
0 0 1 0 1000.0 1000.0 10.0 1000.00
10 120.0
# fi=60 constrained
0.47 1.0 0.000
0 0 1 0 1000.0 1000.0 10.0 1000.00
10 60.0
# fi=60 relaxed
0.47 10.0 0.000
0 0 0 0 1000.0 1000.0 10.0 1000.00
Enter below the number of bonds to monitor and list them in the next line
0
Enter below the number of bends to monitor and list them in the next line
0
Enter below the number of torsions to monitor and list them in the next line
1
10
Enter below the atoms to monitor distances between them and list atoms in the next line
1
2 17
```

File "params.h"

```
parameter (maxgeom = 60)    ! max. number of complexes(geometries) in the fit
parameter (maxparfit= 7)    ! max. number of parameters in the fit
parameter (maxtortct=20)    ! max. number of constrained torsions
logical smithgeom
parameter (smithgeom=.TRUE.)! do not change this one
parameter (maxnch = 1)      ! max. number of chains
parameter (maxatc = 16)     ! max. number of atoms per chain
parameter (maxat = 14)     ! max. number of atoms
parameter (maxbonds = 15)   ! max. number of bonds
parameter (maxbends = 26)   ! max. number of bends
parameter (maxtorts = 27)   ! max. number of torsions
parameter (maxdeforms =1)   ! max. number of deformations
parameter (maxtypes = 5)    ! max. number of nonbonded types
parameter (maxcharges =5)   ! max. number of charge types
parameter (maxbtypes =10)   ! max. number of types for bonds,bends,torsions
.....
C
C  Parameters for the optimizers
C
real*8 TOLX2,GTOL2,STPMX2 ! parameters for geometry-optimizer
logical xcheck2,gcheck2
parameter (TOLX2=1.0d-6)    ! coordinate tolerance
parameter (GTOL2=5.0d-1)    ! gradient tolerance
parameter (STPMX2=0.02d0)   ! maximum Newton step
parameter (xcheck2=.true.)  ! check for coordinate convergence
parameter (gcheck2=.true.)  ! check for gradient convergence
C
real*8 TOLX,GTOL,STPMX     ! parameters for parameter-optimizer
logical xcheck,gcheck
parameter (TOLX=1.0d-3)     ! coordinate tolerance
parameter (GTOL=1.0d-1)     ! gradient tolerance
parameter (STPMX=0.2d0)     ! maximum Newton step
parameter (xcheck=.true.)   ! check for coordinate convergence
parameter (gcheck=.true.)   ! check for gradient convergence
```

File "fort.11" (template) (# sign substitutes word number)

```
NUMBER OF CHAINS+IONS, NUMBER OF IONS
  <total number of polymer chains +ions> <number of ions>
NATCH,NBONDS,NBENDS,NTORTS,NDEFORMS
(this line should be left blank)
<# of atoms> <# of bonds> <#of bends> <# of torsions > <# of out-of plain deformations> for chain 1
<# of atoms> <# of bonds> <#of bends> <# of torsions > <# of out-of plain deformations> for chain 2
<# of atoms> <# of bonds> <#of bends> <# of torsions > <# of out-of plain deformations> for chain 3
.....
<# of atoms> <# of bonds> <#of bends> <# of torsions > <# of out-of plain deformations> for chain n
BONDS (description of bonds)
(this line should be left blank)
  <1st atom of the bond> <2nd atom of the bond> <bond type from fort.12> for bond 1
  <1st atom of the bond> <2nd atom of the bond> <bond type from fort.12> for bond 2
  <1st atom of the bond> <2nd atom of the bond> <bond type from fort.12> for bond 3
.....
  <1st atom of the bond> <2nd atom of the bond> <bond type from fort.12> for bond n
BENDS (description of bends)
(this line should be left blank)
<1st atom of the bend> <2nd atom of the bend> <3d atom of the bend> <bend type from fort.12> for bend 1
<1st atom of the bend> <2nd atom of the bend> <3d atom of the bend> <bend type from fort.12> for bend 2
<1st atom of the bend> <2nd atom of the bend> <3d atom of the bend> <bend type from fort.12> for bend 3
.....
<1st atom of the bend> <2nd atom of the bend> <3d atom of the bend> <bend type from fort.12> for bend n
TORSIONS (description of torsions)
(this line should be left blank)
<1st atom> <2nd atom> <3d atom > <4th atom of the torsion> <torsional type from fort.12> for torsion 1
<1st atom> <2nd atom> <3d atom > <4th atom of the torsion> <torsional type from fort.12> for torsion 2
<1st atom> <2nd atom> <3d atom > <4th atom of the torsion> <torsional type from fort.12> for torsion 3
.....
<1st atom> <2nd atom> <3d atom > <4th atom of the torsion> torsional type from fort.12> for torsion 4
DEFORMS (description of out-of-plain deformations)
(this line should be left blank)
<1st atom> <2nd atom> <3d atom > <4th atom of the deform> <deformation type> <parity> for deform 1
<1st atom> <2nd atom> <3d atom > <4th atom of the deform> <deformation type> <parity> for deform 2
<1st atom> <2nd atom> <3d atom > <4th atom of the deform> <deformation type> <parity> for deform 3
.....
<1st atom> <2nd atom> <3d atom > <4th atom of the deform> <deformation type> <parity> for deform n
```

File "fort.12" (.true. or .false. under the parameter indicates if the parameter is to be fitted or not)

```

*
*      NONBONDED INTERACTIONS
*      <number of nonbonded types>
*~~~~~
*Type(char*3) Charge Polariz A(eq.3-4)      B(eq.3)  C(eq.3-4)      Mass
*~~~~~
cm      <Acm-cm>      <Bcm-cm> <Ccm-cm>      <mass for type cm>
        .false.      .false.  .false.
        <qcm> <αcm>
        .false.
h       <Ah-h>      <Bh-h> <Ch-h>      <mass for type h>
        .false.      .false.  .false.
        <qh> <αh>
        .false.
*      Cross terms for Lennard-Jones and Buckingham potentials
*
cm_h    <Acm-h>      <Bcm-h> <Ccm-h>
        .false.      .false.  .false.
!
*      VALENCE INTERACTIONS
*
*      Bonds (see eq. 6)
*      <number of bond types>
*~~~~~
* Type          K (kcal/mol Å2)      R0(Å)      R0(constrain), not used here
*~~~~~
C_H          <kBONDC-H>      <r0C-H>      1.090
            .false.      .false.
C_C          <kBONDC-C>      <r0C-C>      1.530
            .false.      .false.
*
*      Bends
*      3
*~~~~~
* Type          K(kcal/mol degrees2) A0 (degrees)
*~~~~~
C_C_H          <kBENDC-C-H>      <θ0C-C-H>
            .false.      .false.
H_C_H          <kBENDH-C-H>      <θ0H-C-H>
            .false.      .false.
C_C_C          <kBENDC-C-C>      <θ0C-C-C>
            .false.      .false.
*
*      Torsions (see eq. 8)
*      3
*~~~~~
* Type  # folds  KT0  KT1  KT2  KT3...
*~~~~~
C_C_C_H  4      0.000  0.000  0.000 -0.234
            .false. .false. .false. .false.
H_C_C_H  4      0.000  0.000  0.000 -0.234
            .false. .false. .false. .false.
C_C_C_C  4      0.000  0.340  0.000 -0.630
            .false. .false. .false. .TRUE.
*
*      Out-of-plane deformations
*      0
*~~~~~
* Type          K
*~~~~~

```

File "fort.26"

```
<Comment Line>
<Comment Line>
<Comment Line>
    <x1> <y1> <z1> <atom label from "fort.12"> <charge sub-type from "fort.12">
    <vx1> <vy1> <vz1>
    <x2> <y2> <z2> <atom label from "fort.12"> <charge sub-type from "fort.12">
    <vx2> <vy2> <vz2>
    <x3> <y3> <z3> <atom label from "fort.12"> <charge sub-type from "fort.12">
    <vx3> <vy3> <vz3>
    .....
    <xn> <yn> <zn> <atom label from "fort.12"> <charge sub-type from "fort.12">
    <vxn> <vyn> <vzn>
```

<atom label from "fort.12"> consists from up to 3 characters

<charge sub-type from "fort.12"> is the type of the charge for a given nonbonded type. It could be more than 1 only if the same nonbonded type has a different type, than more than one type is entered in "fort.12"

<v_x_n> <v_y_n> <v_z_n> entered in "fort.26" are ignored

File "fort.50" (output file)

```
#r(phi) Q.C. NB TOT REP DISP LJ COUL IND TB-POL BOND BEND TORT
# <comment line from "tfit.inp" for complex 1>
tort 10 is 180.00 180.00 (is the message indicating that torsion 10 was constrained to the value of 180)
      180.00 0.00 1.35 0.00 5.89 -4.54 1.35 0.00 0.00 0.00 0.06 0.16 -3.18 (energies)
# <comment line from "tfit.inp" for complex 1>
tort 10 is 150.00 150.00 (is the message indicating that torsion 10 was constrained to the value of 150)
      150.00 0.00 0.23 1.46 0.34 -0.12 0.23 0.00 0.00 0.00 0.01 0.09 1.13 (energies)
.....
```

"fort.50" file contains energy contributions for each complex (geometry)

Q.C. is the quantum chemistry energy entered in "tfit.inp" file for this geometry

NB is the nonbonded part of the energy. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the nonbonded energy relative to the first complex is output)

TOT is the total energy (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the first complex the total energy relative to the first complex is output)

REP is the contribution from the repulsion. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the repulsion energy relative to the first complex is output)

DISP is the contribution from the dispersion. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the dispersion energy relative to the first complex is output)

LJ is the sum of repulsion and dispersion energies. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the sum of repulsion and dispersion energies relative to the first complex is output)

COUL is the Coulomb energy. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the Coulomb energy relative to the first complex is output)

IND is the induction energy. (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the induction energy relative to the first complex is output)

TB-POL (usually not used)

BOND is the energy contribution of the bonding potential (eq. 6). (If one of torsional parameters if fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the induction energy relative to the first complex is output)

BEND is the energy contribution of the bending potential. (eq.7) (If one of torsional parameters is fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the bending energy relative to the first complex is output)

TORT is the energy contribution of the torsional potential. (eq.8) (If one of torsional parameters is fit, e.g. .TRUE. is under any torsional parameter, for each complex starting with the second complex the torsional energy relative to the first complex is output)

“fort.62” has a similar output to that of “fort.50”, but it is significantly shortened.

“fort.60” outputs final geometries in the XMOL-XYZ format

“minimum.dat” file contains the optimized parameters

*How to fit torsional and nonbonded parameters?
(coming soon)*