

## Calculating Molecular Coordinates and Intermolecular Geometry and Interaction

The programs are written in FORTRAN, and compiled by gfortran on windows 10.

Step 1. Convert atomic coordinates in cif using trcif.

(In cif, align atoms as S -> C (core) -> C (others) -> H.)

Step 2. Copy the atomic coordinates and the lattice constants to pcal8.dat. Add 6-exp potentials and symmetry operations.

Step 3. Run pcal8. The output file at8.dat contains molecular coordinates, intermolecular geometry, and the 6-exp potentials.

Step 4. Run qcal8. The potential energy is calculated as a function of the dihedral angle.  
(qcal8x changes  $X$  as well.)

Detailed instructions to Step 2.

Example input file of pcal8.dat for BTBT

```

16  ←First 16 atoms are used to define the molecular core.
 1  0.07966 -0.28750  0.14078  S  S  ←Copy the coordinates from at.dat.
 1 -0.07966  0.28750 -0.14078  S  S
 2  0.19290 -0.11460  0.11080  C1 C
 2 -0.19290  0.11460 -0.11080  C1 C
 2  0.31333 -0.16330  0.16945  C2 C
 2 -0.31333  0.16330 -0.16945  C2 C
 2  0.39199 -0.00790  0.13206  C3 C
 2 -0.39199  0.00790 -0.13206  C3 C
 2  0.35164  0.19327  0.03868  C4 C
 2 -0.35164 -0.19327 -0.03868  C4 C
 2  0.23224  0.24316 -0.01810  C5 C
 2 -0.23224 -0.24316  0.01810  C5 C
 2  0.15108  0.08852  0.01762  C6 C
 2 -0.15108 -0.08852 -0.01762  C6 C
 2  0.02488  0.09421 -0.02740  C7 C
 2 -0.02488 -0.09421  0.02740  C7 C
 3  0.33940 -0.30100  0.23370  H2 H
 3 -0.33940  0.30100 -0.23370  H2 H
 3  0.47530 -0.04100  0.17170  H3 H
 3 -0.47530  0.04100 -0.17170  H3 H
 3  0.40750  0.29700  0.01300  H4 H
 3 -0.40750 -0.29700 -0.01300  H4 H
 3  0.20500  0.37600 -0.08050  H5 H
 3 -0.20500 -0.37600  0.08050  H5 H
    ←A blank line defines the end of the atomic coordinates input. *1
S  0.8452  2.15      ←ε and r0 values of the 6-exp potential *2
C  0.2343  1.96
H  0.0837  1.62
11.8009  5.8622  7.9331  90.0000  105.9740  90.0000  ←lattice constants
 1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  1.0  0.0  1.0  0.0  b ←symmetry operation
-1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0 -1.0  0.0  0.5  0.5  p
-1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0 -1.0  0.0 -0.5  0.5  p
 1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  1.0  1.0  0.0  0.0  a
-1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0 -1.0  1.0  0.5  0.5  p ←*3
10.0  ←End of the symmetry operation input
 2  0.11500  0.07  ←Potential map based on SO 2. H and S charges *4
-3.0  3.0  0.5 -3.0  3.0  0.5  3.46  ←Potential map regions *5

```

\*1 If the first number is negative, another set of crystallographically independent atomic coordinates are read from the succeeding lines. The number of atoms should be the same. See pcal8\_pentacene.dat

\*2 Standard 6-exp potentials

**Table 1** Force-field parameters

Atom	$\epsilon$ (kJ mol <sup>-1</sup> )	$r_0$ (Å)	Charge $\rho_i$
C	0.2343	3.92	–
H	0.0837	3.24	0.115
S	0.8452	4.30	0.07
O	0.2466	3.64	–0.30
N	0.1797	3.86	0.00
Se	1.8	4.30	0.07

From <https://dasher.wustl.edu/tinker/distribution/params/>

\*3 If the first number is 5.0, a new set of atomic coordinates (read in \*1) are used for the counter molecule afterwards. See pcal8\_pentacene.dat

\*4 Using the geometry and  $Z$  of the  $n$ -th symmetry, a map of intermolecular potential is created by varying  $X$  and  $Y$ . If this is 30, stacking molecules are investigated. Charges for H, and 1<sup>st</sup>, 2<sup>nd</sup>,... atoms.

\*5 If 3.46→0.0,  $Z$  is taken from the symmetry operation.

Sometimes diagonalization of molecular moments fails, and molecular coordinates are not successfully obtained. Make sure that all core  $Z$  molecular coordinates are almost zero in the at8.dat output. In such a case: (1) Change the atom order. For example, attach S atoms after the core C atoms. (2) Decrease the core atom number. For example, exclude the terminal rings. Note that the molecular center may change depending on the eliminated atoms.