

# SCAL

## Calculation of Intermolecular Overlap Integrals

By using the results of molecular orbital calculation `extdh`, we can estimate the transfer integrals. Here we assume the transfer integrals  $t$  are proportional to the intermolecular overlap integrals  $S$  as  $t = ES$ , where  $E$  is a constant in the order of the energy of the molecular orbital, so we usually take as  $E = -10$  eV. Then the estimation of intermolecular overlap integrals is equivalent to the estimation of transfer integrals.

This program calculate intermolecular overlap integrals on the basis of extended Hückel molecular orbital calculation.

Input data:    `scal.dat`  
Source:        `scal.f`  
Indy:         `scal.out`  
PC:            `scal`

This program generates the following output file:

Output:        `sdat.dl`

## Test Data

The supplied input files are for 1-(BETS)<sub>2</sub>FeCl<sub>4</sub>.

- (1) Download `scal.dat` and the `scal` executable program suitable for your computer.
- (2) Prepare `fort.10` and `fort.20` according to `extdh.doc`.
- (3) Run `scal`. This program reads data from `fort.10` and `fort.20` as well as `scal.dat`. This program generates `sdat.dl`. Open `sdat.dl`, and check the calculation is OK.

First calculate HOMO of donors, and LUMO of acceptors by `extdh`. The program `scal` reads the coefficient from `fort.10`. Other input data are quite similar to `extdh.dat`. Before starting the editor, prepare a figure which shows the donor arrangement in the conducting sheet. We usually use a figure that is seen along the molecular long axis. Then specify the original molecule which is given in `extdh.dat`. This is easily done by obtaining the center of gravity from the midpoint of the central C=C bond. Next specify the adjacent molecules which are generated by some kinds of symmetry operations and/or translations. It is frequently necessary to consult International Table for Crystallography to obtain the form of the symmetry operations.

## Input Data

The following is an example of input data in `scal.dat`.

```
5  6  6  0  0 B-(BEDT-TTF)2IBR2
26  1
1  0.4663 -0.2595  0.4475      S1
1  0.1029 -0.1444  0.4277      S2
```



```

2 2 1
2 2 2
3 1 2
4 2 1

```

```

Line 1 5 0 6 (3I5)
5: Input file number that is opened as "scal.dat".
0: Output of coefficients and rectangular coordinates.
6: Output file number that is opened as "sdat.dl".
Line 2 26 1 (2I4)
Number of atoms. The next 1 is not used in the program.
Line 3 1 0.4663 -0.2595 0.4475 (I4, X, 3F10.5) x26
Atom species defined by Line 5 and its x, y, and z coordinates. Atom names are not
used inside, but are recommended to be written for your memory.
Line 4 1 Blank line
Line 5 S 3 16 10 (A4, 3I4)
Sulfur atom has three kinds of orbitals which are defined by the next lines.
16 and 10 are the numbers of total and core electrons, but these numbers are not
used inside the program.
Line 6 3 0 2.122 -1.47 (2I4, 3F10.0) x3
3: principal quantum number.
0: azimuthal quantum number 0 is s, 1 is p and 2 means d orbitals.
2.122 is Slater exponent z, and
-1.47 is ionization potential in Ryd (-13.6 eV).
These values are taken from the previous literatures.3-5 z =0.0 means double or
triple zeta, and requires the next line.
Line 6' (I4, X, 6F10.5) only when z =0.0.
Double z : 2 z 1 c1 z 2 c2
Triple z : 2 z 1 c1 z 2 c2 z 3 c3
Line 7 1 Blank line
Repeat Lines 5 - 7 with the number of atom species.
Line 8 1.75 0.01 1 (3F10.0)
Coefficient of extended Hückel equation. Usually 1.75.
Line 9 6.593 8.975 15.093 93.790 94.970 110.540 (6F10.5)
Lattice constants. a, b, c, a, b, and g. When the angles are 90°, the columns
may remain blank.
Line 10 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0
(12F5.0) xNUNIT

Symmetry operations
(x') (CK(1) CK(2) CK(3)) (x) (CK(10))
(y') = (CK(4) CK(5) CK(6)) (y) + (CK(11))
(z') (CK(7) CK(8) CK(9)) (z) (CK(12))
When CK(1) ≥ 10.0, proceed to the next line.
Line 11 120 1 10 (5I5)
120: The number of orbitals on a molecule. This number should be the same as that
calculated in EXTDH (1). [Not used in scalg]
1: Coefficients of one molecule are read from fort.10. If there are more than two
independent molecules, change this line like
120 2 10 20

```

After the NCELL ( $\leq 6$ ) molecules are read from fort.10, fort.20, etc, these molecules are duplicated by the symmetry operations given in Line 10. If NUNIT symmetry operations are read from Line 10, the total number of molecules are NCELL x NUNIT. Then the unit cell contains NCELL x NUNIT molecules.

Line 120.0 0.0 0.0 (3F5.0)

Translation that is applied to the molecules in Line 11.

When  $x \geq 10.0$ , proceed to the next line.

Line 133 1 2 (3I5)

Calculate the overlap integral between the first molecule in the original cell and the second molecule in the cell generated by the third translation (Line 12). End of calculation if the first number is zero.

To understand this example, see Figure in beta.gif.

- (3) Move the lattice constants to the proper position.
- (4) Edit Lines 10-13 by following the above instructions.

As another way, it is also easy to prepare scal.dat from extdh.dat. To do so:

- (1) Copy extdh.dat to scal.dat. For Indy,  
cp extdh.dat scal.dat
- (2) Move the lattice constants to Line 9, and delete the former two lines:  
0 48 0 10  
96.
- (3) Delete the last line  
1  
and add Lines 10-13.

Finally run the program, and check the output file, sdat.d1.