

DCAL

Calculation of Intermolecular Overlap Integrals for p d Sytem

This program calculate intermolecular overlap integrals between different species such as donor and anions on the basis of extended Hückel molecular orbital calculation.

Input data: dcal.dat
Source: dcal.f
Indy: dcal.out
PC: dcal

This program generates the following output file:

Output: ddat.dl

Test Data

The supplied input files are for 1-(BETS)₂FeCl₄.

- (1) Download scal.dat and the scal executable program suitable for your computer.
- (2) Prepare fort.10, fort.20, and fort.30 according to extdh.doc.
- (3) Run dcal. This program reads data from fort.10, fort.20, and fort.30 as well as dcal.dat. This program generates ddat.dl. Open ddat.dl, and check the calculation is OK.

Input Data

The input data are mostly the same as scal.dat. The following are example for 1-(BETS)₂FeCl₄.

```
5 99 6 0 0 1-(BETS)2FeCl4
57 1
1 0.58579 -0.01733 -0.31480 SE1
1 0.58837 -0.07773 0.10960 SE2
1 0.73889 0.16444 -0.07360 SE3
1 0.74782 0.10768 0.35490 SE4
2 0.44880 -0.17670 -0.56190 S1
2 0.44720 -0.24470 -0.09390 S2
2 0.86100 0.33560 0.12060 S3
2 0.88010 0.27420 0.59370 S4
3 0.63460 0.00660 -0.02600 C1
3 0.50950 -0.12460 -0.31500 C2
3 0.51000 -0.14990 -0.13200 C3
3 0.37450 -0.26750 -0.50700 C4
3 0.39630 -0.29940 -0.35000 C5
3 0.69670 0.08040 0.06900 C6
3 0.81310 0.24000 0.17000 C7
```

3	0.81740	0.21600	0.35200	C8
3	0.93290	0.39380	0.37000	C9
3	0.89110	0.37140	0.55300	C10
4	0.32112	-0.26014	-0.48339	H1
4	0.36023	-0.30680	-0.63064	H2
4	0.43681	-0.32172	-0.39446	H3
4	0.34102	-0.34098	-0.33877	H4
4	0.98819	0.38651	0.38099	H5
4	0.94572	0.44848	0.37324	H6
4	0.83207	0.37166	0.53275	H7
4	0.92801	0.41004	0.67424	H8
1	0.13080	0.02414	-0.18700	SE5
1	0.12790	-0.03323	0.24200	SE6
1	0.28438	0.20687	0.05550	SE7
1	0.28211	0.15136	0.48910	SE8
2	-0.02260	-0.13070	-0.42130	S5
2	-0.02970	-0.19330	0.04750	S6
2	0.41970	0.37940	0.28180	S7
2	0.42280	0.31640	0.72210	S8
3	0.17810	0.05130	0.10200	C11
3	0.04470	-0.07850	-0.17900	C12
3	0.04270	-0.10160	0.00200	C13
3	-0.08500	-0.22780	-0.37600	C14
3	-0.05120	-0.25420	-0.20300	C15
3	0.23970	0.12450	0.19900	C16
3	0.35950	0.28060	0.29900	C17
3	0.35930	0.25720	0.48300	C18
3	0.38450	0.42240	0.50600	C19
3	0.43040	0.41600	0.71000	C20
4	-0.14354	-0.23050	-0.35832	H9
4	-0.09099	-0.26485	-0.49854	H10
4	0.00435	-0.25736	-0.22612	H11
4	-0.09489	-0.30587	-0.20150	H12
4	0.39943	0.47719	0.50581	H13
4	0.32040	0.39503	0.49316	H14
4	0.40296	0.43216	0.81760	H15
4	0.49306	0.45108	0.73334	H16
5	0.20965	0.46665	0.88070	FE1
6	0.09180	0.46920	1.00510	CL1
6	0.21560	0.35150	0.89010	CL2
6	0.33730	0.56180	1.05320	CL3
6	0.19320	0.47740	0.55300	CL4

SE	3	16	10	
4	0	2.44	-1.4706	
4	1	2.07	-0.7941	
4	2	1.5	-0.4	

S	3	16	10	
3	0	2.122	-1.4706	

3 1 1.827 -0.8088
3 2 1.5 -0.4

C 2 6 2
2 0 1.625 -1.573
2 1 1.625 -0.838

H 1 1 0
1 0 1.0 -1.0

Fe 3 16 10
4 0 1.9 -0.6743
4 1 1.9 -0.3948
3 2 -0.9338
2 5.35 0.5366 1.80 0.6678

Cl 2 6 2
3 0 2.033 -2.206
3 1 2.033 -1.103

1.75 0.01 1
16.164 18.538 6.5928 98.40 96.67 112.52
1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0
-1.0 0.0 0.0 0.0 -1.0 0.0 0.0 0.0 -1.0 0.0 0.0 0.0

10.0

120 2 10 20
25 5 2 1 30

0.0 0.0 0.0
1.0 1.0 1.0
-1.0 0.0 1.0
0.0 1.0 1.0
1.0 1.0 2.0
-1.0 0.0 0.0
0.0 1.0 2.0
0.0 0.0 1.0
0.0 0.0 -1.0

10.0

1 3 2
1 3 5
2 3 4
3 3 1
4 3 1
5 3 4
5 3 5
6 3 1
7 3 1
8 3 5
8 3 2
9 2 3
7 3 6

8 3 3

The only difference from scal.dat is that the following second line should be added next to the first line as for the input of molecular orbital coefficients.

```
120  2  10  20
25   5   2   1  30
```

Line 11 120 2 10 20 (5I5) Input p -orbitals
120: The number of orbitals on a molecule. This number should be the same as that calculated in EXTDH (1).

2: Coefficients of one molecule is read from fort.10 and fort.20.

Line 11' 25 5 2 1 30 (5I5)

25: The number of orbitals on the FeCl_4^- molecule stored in fort.30. From this, 5 d-energy levels are read, and the sums are separately calculated for the first (lower) 2 levels (e_g), and consequently the remaining upper 3 (t_{2g}) levels. There are crystallographically independent 1 anion(s), whose coefficients are read from fort.30.

The molecules are arranged in the order of 1: A (fort.10), 2: B (fort.20), and 3: FeCl_4^- (fort.30), and those which are moved by a symmetry operation ($-x, -y, -z$) (Line 10 defined by

```
-1.0 0.0 0.0 0.0 -1.0 0.0 0.0 0.0 -1.0 0.0 0.0 0.0)
```

are 4: A, 5: B, and 6: FeCl_4^- . Then Line 13

```
1 3 2
```

indicates to calculate intermolecular overlap from the molecule number 3 (original FeCl_4^-) to the molecule number 2 (original B molecule). Similarly, the line

```
2 3 4
```

represents intermolecular overlap from the original FeCl_4^- to the molecule number 4 (B molecule moved by $(-x, -y, -z)$ and the 2-nd translation (1.0 1.0 1.0) (namely (1-x, 1-y, 1-z) as a whole). The output results are for independent five d-levels, and the root of the square sum $\sqrt{\sum t^2}$ for e_g and t_{2g} sets as well as the total sum.