

PLANEA

Geometry of Molecules

To analyze the geometry of two molecules that give the overlap integrals, define the "molecular coordinates" and calculate "x, y, z, and f".

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

This program generates the following output file:

Output: padat.dl

For Mac, old version "plane" is supplied. Change the input filename to "plane.dat."

Otherwise, the input data are the same. This program does not calculate the dihedral angle. The output filename is pdat.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) Run planea, and check padat.dl.

Input Data

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

```
5 99 6 0 0 (BEDT-TTF)2KHG(SCN)4 298 K
14 1
10.082 20.565 9.933 103.700 90.91 93.060
2 0.9730 0.4678 0.4860 C5 B
2 1.0270 0.5321 0.5140 C6 B
1 1.0346 0.4056 0.5562 S3 B
1 1.1668 0.5576 0.6244 S5 B
1 0.8332 0.4424 0.3756 S4 B
1 0.9654 0.5944 0.4438 S6 B
1 0.9500 0.2615 0.4877 S1 B
1 1.2964 0.6917 0.7182 S7 B
1 0.7036 0.3083 0.2818 S2 B
1 1.0500 0.7385 0.5123 S8 B
2 0.9206 0.3413 0.4650 C3 B
2 1.1682 0.6410 0.6163 C8 B
2 0.8318 0.3590 0.3837 C4 B
```


way we can estimate all A-A and A-B geometries, but we cannot obtain the geometries of B-B interactions. To calculate these interactions, input the coordinates of the B molecule from the first, and run the program again.

Lines 1 to 3 are the same as `extdh.dat`. Rearrange the order of the atoms, and after those, newly write Lines 5 and 6.

After saving the results to `planea.dat`, run the program, and see the output, `padat.dl`