## 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. d1

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 $1-(\mathrm{BETS})_{2} \mathrm{FeCl}_{4}$.
(1) Download scal. dat and the scal executable program suitable for your computer.
(2) Run planea, and check padat. d1.

## Input Data

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



Line $1 \quad 5 \quad 99 \quad 6$
5: Input file number that is opened as "planea. dat".
99: Not used.
6: Output file number that is opened as "padat. d 1 ".
Line 2141
Number of atoms. Only input the atoms that define the molecular plane following Figure, ET. gif, so this number is 6,10 or 14 .
1 is not used.
Line $3 \quad 10.082 \quad 20.565 \quad 9.933 \quad 103.700 \quad 90.91 \quad 93.060$ (6F10.5)
Lattice constants. a, b, c, a , b , and g . When the angles are $90^{\circ}$, the columns may remain blank.
Line $420.9730 \quad 0.4678 \quad 0.4860 \quad$ (I4, X, 3F10.0)
Atomic coordinates. The atoms must be arranged in the order of Figure in ET. gif.
Line $5 \quad 5$
(I5)
The number of symmetry operations read in the next lines 6 .
Line 61.00 .00 .00 .01 .00 .00 .00 .01 .00 .01 .00 .0
(12F6. 0)
Symmetry operations


The computer calculates the molecular coordinates of the original molecule, and after this symmetry operation, the position of the moved molecule is calculated and represented by the "molecular coordinates".
If there are more than two crystallographically independent molecules, we have to input the second molecule. In that case input CK (1) $\geq 20.0$, and new atomic coordinates are read after the input of Line 6 . After once $C K(1) \geq 20.0$ appears, the coordinates of the moved molecule are generated from the new coordinates. In this
way we can estimate all $\mathrm{A}-\mathrm{A}$ and $\mathrm{A}-\mathrm{B}$ 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. d1

