## 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  $1 - (BETS)_2 FeCl_4$ .

- (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	(BEDI	[-]	TF) 2KH	IG (SCN)	4	298	Κ		
14	1												
10.08	2	20.	565	9.	. 933		103.	700	90.	91		93.0	)60
2	0.9	9730	0.	4678	8	0.	4860		C5	В			
2	1.0	270	0.	532	1	0.	5140		C6	В			
1	1.0	)346	0.	405	6	0.	5562		S3	В			
1	1.1	668	0.	557	6	0.	6244		S5	В			
1	0.8	3332	0.	4424	4	0.	3756		S4	В			
1	0.9	654	0.	594	4	0.	4438		S6	В			
1	0.9	9500	0.	261	5	0.	4877		S1	В			
1	1.2	2964	0.	691	7	0.	7182		S7	В			
1	0.7	'036	0.	308	3	0.	2818		S2	В			
1	1.0	)500	0.	738	5	0.	5123		S8	В			
2	0.9	206	0.	3413	3	0.	4650		C3	В			
2	1.1	682	0.	641	0	0.	6163		C8	В			
2	0.8	318	0.	359	0	0.	3837		C4	В			

C7 B 2 1.0794 0.6587 0.5350 5 1.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0 1.0 0.0 0.0 1.0 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0 1.00.0 20.0 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 1.0 0.0 0.0 1.0 2 0.4581 0.4696 0.2450 C52 0.5133 0.5337 0.2795 С6 0.1881 0.3082 0.2721 S1 1 1 0.5479 0.7381 0.4951 **S7** S2 1 0.4470 0.2641 0.0401 0.7892 0.6912 0.2423 S8 1 1 0.3146 0.4431 0.3183 S3 1 0.4508 0.5964 0.4087 S5 0.5254 0.4085 S4 1 0.1165 1 0.6525 0.5583 0.1978 S6 2 0.3194 0.3588 0.2293 С3 2 0.5694 0.6592 0.3894 C8 2 0.4171 0.3430 0.1369 C4 2 0.6611 0.6424 0.2920 C7 Line 1 5 99 6 (3I4)5: Input file number that is opened as "planea.dat". 99: Not used. 6: Output file number that is opened as "padat.dl". (214)Line 2 14 1 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 10.082 20.565 9.933 103.700 90.91 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 4 2 0.9730 0.4678 0.4860 (I4, X, 3F10.0) Atomic coordinates. The atoms must be arranged in the order of Figure in ET.gif. Line 5 5 (I5)The number of symmetry operations read in the next lines 6. Line 6 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0 1.0 0.0 (12F6.0)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))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  $CK(1) \ge 20.0$ , and new atomic coordinates are read after the input of Line 6. After once  $CK(1) \ge 20.0$  appears, the

coordinates of the moved molecule are generated from the new coordinates.

In this

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