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APPENDICES

Appendix I

GENERATE version 1.0

Program Manual

Program ***GENERATE*** version 1.0 was developed to generate and calculate complexation energy for the development of intermolecular pair potential function. The source code has been written in Fortran language using FORTRAN-77. This compact manual provided step-by-step instrutions, and demonstration with an example of input and/or output in an easy understanding.

The program structure of Main program is shown in Figure A.1.

```
Program Main
CALL Read_Input()

CALL Generate_Configuration()

IF(method.EQ.1)THEN
  CALL Without()
ELSE
    IF(method.EQ.2)THEN
      CALL With_BSSE()
    ELSE
        IF(method.EQ.3)THEN
          CALL Without()
          CALL With_BSSE()
        ELSE
          CONTINUE
        END IF
    END IF
END IF

STOP

END
```

Figure A.1 Procedural detail of Main program.

Running the *GENERATE* Program

If you have the source code of ***GENERATE*** program, you should first compile the ***GENERATE*** program by FORTRAN-77 (see the compile procedures in the manual of FORTRAN-77). In the other hand, if you already have execute file, i.e. ***GENERATE_OUT***, you can run the program by typing ***GENERATE_OUT*** in the UNIX promt as:

```
$ GENERATE_OUT
```

1) *Subroutine Read_Input*

This routine reads all information from the input file and keep them for processing.

2) *Subroutine Generate_Configuration*

This routine gets the input from subroutine ***Read_Input***. Then, numerous position of molecule B around A can be automatically generated.

3) The *ab initio* calculation

The program is designed to calculate interaction energy for the following 3 choices: either with or without BSSE corrections or both.

Appendix II

1. Input file for NH_3-Li^+

```
3
#RHF
d95**
1 1

4
0 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470

1
1 1
Li     0.000000     0.000000     0.000000

4
1.5  1.7  0.1
1.7  3.0  0.05
3.0  6.0  0.5
6.0 10.0  2.0

0   180
0    60
30
30

0      0
0      0
0      0
0
0
0
```

2. Input file for NH_3-NH_3

```
3
#RHF
d95**
0 1

4
0 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470

4
0 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470

4
2.4    3.0   0.2
3.0    4.0   0.1
4.0    6.0   0.5
6.0   10.0   2.0

0      0
0      0
30
30

0     60
60    60
30    30
30
30
30
```

3. Output file for NH_3-Li^+

alpha=0	beta=0	gamma=0	theta=0	phi=0
53.370		0.000000	0.000000	1.300000
-7.752		0.000000	0.000000	1.500000
-23.055		0.000000	0.000000	1.600000
-32.425		0.000000	0.000000	1.700000
-35.510		0.000000	0.000000	1.750000
-37.775		0.000000	0.000000	1.800000
-39.366		0.000000	0.000000	1.850000
-40.403		0.000000	0.000000	1.900000
-40.986		0.000000	0.000000	1.950000
-41.200		0.000000	0.000000	2.000000
-41.113		0.000000	0.000000	2.050000
-40.785		0.000000	0.000000	2.100000
-40.263		0.000000	0.000000	2.150000
-39.588		0.000000	0.000000	2.200000
-38.794		0.000000	0.000000	2.250000
-37.910		0.000000	0.000000	2.300000
-36.958		0.000000	0.000000	2.350000
-35.959		0.000000	0.000000	2.400000
-34.928		0.000000	0.000000	2.450000
-33.879		0.000000	0.000000	2.500000
-32.823		0.000000	0.000000	2.549999
-31.768		0.000000	0.000000	2.599999
-30.721		0.000000	0.000000	2.649999
-29.690		0.000000	0.000000	2.699999

4. Output file for NH_3-NH_3

```
alpha=0 beta=60 gamma=30 theta=0 phi=0
  26.725          0.000000    0.000000    2.400000
                  0.812124    0.564803    2.615327
                 -0.000002   -0.138516    1.397144
                 -0.812122    0.564801    2.615324
  11.065          0.000000    0.000000    2.600000
                  0.812124    0.564803    2.815327
                 -0.000002   -0.138516    1.597144
                 -0.812122    0.564801    2.815324
   3.187          0.000000    0.000000    2.800000
                  0.812124    0.564803    3.015327
                 -0.000002   -0.138516    1.797144
                 -0.812122    0.564801    3.015324
  -0.507          0.000000    0.000000    3.000000
                  0.812124    0.564803    3.215327
                 -0.000002   -0.138516    1.997144
                 -0.812122    0.564801    3.215324
  -1.449          0.000000    0.000000    3.100000
                  0.812124    0.564803    3.315327
                 -0.000002   -0.138516    2.097144
                 -0.812122    0.564801    3.315324
  -2.017          0.000000    0.000000    3.200000
                  0.812124    0.564803    3.415327
                 -0.000002   -0.138516    2.197144
                 -0.812122    0.564801    3.415324
  -2.325          0.000000    0.000000    3.300000
                  0.812124    0.564803    3.515327
                 -0.000002   -0.138516    2.297144
                 -0.812122    0.564801    3.515324
  -2.458          0.000000    0.000000    3.400000
                  0.812124    0.564803    3.615327
                 -0.000002   -0.138516    2.397144
                 -0.812122    0.564801    3.615324
  -2.477          0.000000    0.000000    3.500000
                  0.812124    0.564803    3.715327
                 -0.000002   -0.138516    2.497144
                 -0.812122    0.564801    3.715324
  -2.423          0.000000    0.000000    3.600000
                  0.812124    0.564803    3.815327
                 -0.000002   -0.138516    2.597144
                 -0.812122    0.564801    3.815324
  -2.325          0.000000    0.000000    3.700000
                  0.812124    0.564803    3.915327
                 -0.000002   -0.138516    2.697144
                 -0.812122    0.564801    3.915324
  -2.204          0.000000    0.000000    3.800000
                  0.812124    0.564803    4.015327
                 -0.000002   -0.138516    2.797144
                 -0.812122    0.564801    4.015324
  -2.071          0.000000    0.000000    3.900000
                  0.812124    0.564803    4.115327
                 -0.000002   -0.138516    2.897144
                 -0.812122    0.564801    4.115324
```

5. Basis Set Superposition Error: Li^+ as a Ghost Atom

```
#RHF/d95**      Massage

g98

1 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470
Li     0.000000     0.200000     0.000000

 5 0 0.0
```

6. Basis Set Superposition Error: NH_3 as a Ghost Atom

```
#RHF/d95**      Massage

g98

1 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470
Li     0.000000     0.200000     0.000000

 1 0 0.0
 2 0 0.0
 3 0 0.0
 4 0 0.0
```

7. Basis Set Superposition Error: For the complex

```
#RHF/d95**      Massage

g98

1 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470
Li     0.000000     0.200000     0.000000
```

8. Basis Set Superposition Error: NH_3 (molecule B) as a Ghost Atom of NH_3-NH_3 system

```
#RHF/d95**      Massage

g98

0 1
N      0.000000     0.000000     0.000000
H      0.937760     0.000000    -0.381470
H     -0.468880    -0.812120    -0.381470
H     -0.468880     0.812120    -0.381470
N      0.000000     0.000000    10.000000
H     -0.083072     0.985721    10.215327
H      0.119957    -0.069259     8.997144
H     -0.895193    -0.420918    10.215324

 5 0 0.0
 6 0 0.0
 7 0 0.0
 8 0 0.0
```

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