

Input Preparation Guide for the Program CINDO.x

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All the input data is written in the free format to minimize errors. Therefore, before each important input card, there is a compulsory comment line to make the input self explanatory. It is irrelevant as to what is written in the comment lines, but, by writing something meaningful, one can keep the input process transparent. We do require that all the ASCII input cards (not the ones in the comment lines) should be in uppercase letters. To distinguish comment lines from the input, in this guide we precede each comment line with the character '#', although in actual input files, that is seldom done. We encourage the user to compare the explanation provided here with the actual input files provided in the Examples subdirectory. Next, we explain the preparation of input files card by card.

1. As our code has been framed to handle for the molecules and clusters, the first input card will read the total number of atoms in a given molecule or cluster, followed by the comment line.

For example, if we are handling a system having two number of atoms in all, then the first card will read

```
# Total number of atoms in the molecules/clusters  
2
```

2. The second card will read the nuclear charge on each atom of the molecule. The magnitude of the nuclear charges have been defined as real variables.

For example, in case of a lithium hydride molecule, the card will read as follows

```
#Nuclear charges of the atoms  
1.0,3.0
```

3. The third card deals with the Cartesian coordinates of the different atoms of the molecules. The coordinate values are usually in Å. However, in the program, the values have been converted into atomic units. One thing is important to note here that the order of the atoms whose coordinates

are to be specified, should be of the same order as nuclear charges in the previous card.

For example, for the same lithium hydride molecule, a typical coordinate systems have been supplied as input as follows,

```
# Position of the nuclei
0.0 ,0.0 ,0.0
0.0 ,0.0 ,1.573d0
```

4. The fourth card is an ASCII card describing the model Hamiltonians to be used for the system. Options are: CNDO, INDO.

(a) For a system using CNDO model, the input card may read:

```
# The Hamiltonian to be used
CNDO
```

(b) For a system using INDO model, the input card may read:

```
# The Hamiltonian to be used
INDO
```

5. The fifth card is also an ASCII card that specifies the type of SCF calculation to be performed over the system. Options are: RHF for restricted Hartree-Fock method and UHF for unrestricted Hartree-Fock method. In case of UHF, the card then immediately reads the number of up-spin and down-spin electrons respectively.

If unrestricted Hartree-Fock calculation, for example, to be performed over a system having four spin-up and two spin-down electrons, the input may be;

```
# Type of calculation to be performed
UHF
4, 2
```

6. The sixth card reads if the system is neutral or ionic. For a neutral system 0 is used while for a single anion -1 is used and so on.

For example, in case of any neutral system, the input reads as;

```
# Ionic state of the system
0
```

7. The seventh card reads the convergence threshold, followed by the maximum number of iterations allowed to achieve convergence. Thus, for a convergence threshold of 1.0×10^{-7} units on total energy, with the maximum 100 iterations allowed, the input will be

```
# SCF convergence threshold, Maximum iterations allowed
1.d-7,100
```

8. Sometimes, because of some damping, it becomes difficult to achieve convergence. However in those cases one usually utilizes the techniques of Fock matrix mixing or orbital mixing. In our program we have the technique of only Fock matrix mixing. So we have two options; (a) DAMP for Fock matrix mixing (b) NODAMP for no mixing. In case option(a) is chosen, one needs to specify the parameter *xdamp* quantifying the mixing according to the formula

$$R^{(i)} = xdamp R^{(i)} + (1 - xdamp) R^{(i-1)}$$

where $R^{(i)}$ is the quantity under consideration in the i-th iteration. Thus, if Fock matrix mixing is allowed, *xdamp* specifies the fraction of the new Fock matrix in the total Fock matrix in the i-th iteration.

For example, if in the calculation, no Fock matrix mixing is allowed, then the input file reads,

```
# If damping to be taken into account
NODAMP
```

9. The ninth card specifies if Mulliken charge of the system is to be specified. The option is MULLIK. So the input format is like,

```
#Mulliken population analysis
MULLIK
```

10. The tenth card describes whether the user wants the numerical values of the orbitals/densities along user specified set of data points, such that they could be plotted as a function of spatial coordinates. The output of this module is written in a file called *orb_plot.dat* which can be used to visualize the orbitals/densities. The options are: ORBPLT(for orbital plotting), DENPLT(for density plotting), BOTHPLT(for both orbital and density plotting) and NOPLT(to disable the plotting option). In addition, for the plotting of density one can optionally print out the log10 of the density which can be useful in making contour plots. Keyword DENPLT have then to be followed options such as 1D, 1DLOG, or 2D, 2DLOG. However in case of ORBPLT, option like 1D or 2D will be allowed depending upon the plotting to be linear or planer respectively. If 1D PLOT has been opted, further data *rmin*, *rmax*, *dr* is specified next which determines the starting position, ending position, and the step size for generating the points on which the condensate is to be computed. After these values, we need to specify variable *ndir* which is the number of directions along which the orbital/density needs to be computed. For the case of 2D plots, one has to supply: (a) range of values of two Cartesian coordinate in the plane in the order *xmin*, *xmax*, *dx*, followed by *ymin*, *ymax*, *dy* (note that variable names *x*, and *y* here are generic, and will correspond to any two coordinates which characterize the plane. This is followed by the variable *nplane*, which represents number of planes on which the plots are needed, (b) for each of the planes, the Cartesian axis

(variable *iaxis*) which is perpendicular to the plane, and (c) The location of each of these planes in terms of the value of the constant Cartesian coordinate along the plane (variable *zval*). Next, one has to specify as to how many, and which, orbitals will be plotted. So for RHF case, one has to specify the value of variable *nplot*. If *nplot* < 0, then it is assumed that all the occupied orbitals will be plotted and no further input is needed. However, if *nplot* > 0, then *nplot* values of the orbital indices have to be provided. For UHF case, one has to first provide the values of two variables *nplot - u*, and *nplot - d*, corresponding to the up- and down-spin orbitals, respectively. However additionally, one has to specify which orbitals are to be plotted, in form. We consider various input scenarios below.

(a) If we want to plot all the occupied orbitals of RHF calculation in the range of -5.0 to 5.0 in the step of 0.5, along one direction (0,0,1), then the input format is

```
# Plotting of orbital
ORBPLT
1D
-5.d0, 5.d0, 0.5d0
1
0 0 1
-2
```

(b) However, if we want to plot orbitals number 1, 2, and 4 with the range and direction as above, the input is

```
#Plotting of orbitals
ORBPLT
1D
-5.d0, 5.d0, 0.5d0
1
0 0 1
3
1,2, 4
```

(c) For 1D plotting of UHF calculations, if all the occupied orbitals or specific numbered orbitals to be plotted, is specified for both spin-up and spin-down electrons. For example if orbitals number 1,3,5 corresponding spin-up electrons and orbital number 3,5,7,9 corresponding spin-down electrons to be plotted, the input format is,

```
#Plotting of orbitals
ORBPLT
1D
-5.d0, 5.d0, 0.5d0
1
0 0 1
```

3,4
1,3, 5
3,5,7,9

(d) If, however we want to plot for ,say density, in a plane which is decided by a variable *iaxis*, then we have to supply the the ranges of the two axes forming the plane and a value to the third axes. The input reads that value as the variable *zval* which is put just after *iaxis*.

For example, if we need to plot density for all occupied orbitals in an *xy*-plane, then the input format is

```
#Plotting of orbitals
DENPLT
2D
-5.d0, 5.d0, 0.5d0
-5.d0, 5.d0, 0.5d0
1
3
0.0
-1
```

(e) In case of 2D plotting for UHF calculations, if spin-up orbital #1,2,3 and spin-down orbital # 3,5 to be plotted in *xy*- (in a range -5.0 to 5.0) and *yz*-planes (with a range -5.0 to 5.0) respectively with certain values for their respective perpendicular axes, the input will be as follows

```
#Plotting of orbitals
DENPLT
2D
-5.d0, 5.d0, 0.5d0
-5.d0, 5.d0, 0.5d0
2
3, 1
0.0, 1.0
3,2
1,2,3
3,5
```

11. This input card will facilitate the user through an option DIPOLE for if he/she needs to calculate the dipole moment of the molecule. If dipole moment is not required, the option is then NODIPOLE. So the input is

```
# Dipole moment calculation
DIPOLE For no dipole moment calculation, the input is
```

```
# Dipole moment calculation
NODIPOLE
```

12. This input card deals with the calculation of linear optical absorption, and is applicable only for RHF calculations. If the optical absorption calculation is needed, one has to supply the keyword OPTICS followed by $d\omega, \omega_{min}, \omega_{max}, \Gamma$, where $d\omega$, represents the frequency step, $\omega_{min}/\omega_{max}$ represent minimum/maximum range of frequencies for which the spectrum is to be computed, while Γ is the line width of the excited states. The out put of these calculation has been written in a file named *spectrum.dat*. The input format is

```
# Linear Optical Absorption Calculation
OPTICS
0.25, 0.0, 10.d0, 0.01, 1.d0
```