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Version: Aug. 16, 2012


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Input parameters
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(1)   Information of molecule

2         read (*,*) n_atom
                     How many atoms
1         read (*,*) n_mode
                     How many modes

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(2)   Random number generations


0         read (*,*) label_random
                     0: Do not generate the random numbers.
                        In this case, any number can be defined
                        in the next two lines in the input file.
                     1: Generate the random number a 2D Gaussian
                        distribution (X,Y)
                        In this case, the code will read the
                        parameter of nr and nbin from next two lines.
1000      read (*,*) nr
                     how many pair of random numbers?
50        read (*,*) nbin
                     If we wish to plot the distribution of
                     random numbers, this term is needed.
                     The code will find the X_min and X_max.
                     Then the window is defined as
                     dx = (X_max-X_min) / nbin

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(3)   Read the normal modes

1                 read (*,*) label_read_vib
                    0:  Do not read the normal modes
                    1:  Read the normal modes.

1                 read (*,*)  label_es_output
                    1: Read Molden file generated from MNDO calculations
                    2: Read Turbomole output
                    3: Read Gaussian output (Single frequency calculations with the
option "HPmode").
molden.molf       read (*,*)  filename_es_output
                    Define the filename which includes the equilibrium geometry and
normal modes.
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(4)   Generate the geometries along the dimensionaless normal
      coordinate. For each dimensionaless normal coordinate Q_i,
      eleven points with equal space are generated between
      -2 < Q_i < 2 with step size 0.2.
      (Q_i = [-1:0.2:2])
      Then transform Q_i to the Catersian coordinate to obtain
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      the corresponding structures.

1         read (*,*) label_displacement
                     0: Do not create the Q_i within -2 < Q_i < 2.
                     1: Generate Q_i within -2 < Q_i < 2.

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(5)   Generate the geometries along the dimensionaless normal
      coordinate. For each dimensionaless normal coordinate Q_i,
      the wigner distribution [ N exp(-Q_i**2-P_i**2) ]
      is used to generate the  Q_i and P_i

0         read (*,*) label_dis_wigner
                     0: Do not generate Q_i from Wigner distribution.
                        In this case, any number can be defined
                        in the next two lines in the input file.
                     1: Generate Q_i from Wigner distribution.
                        In this case, the code will read the
                        parameter of n_geom and label_method
                        from next two lines.

100       read (*,*) n_geom
                     How many geometries?
1         read (*,*) label_method
                     How to generate the P_i
                     1: From Wigner distribution.
                     2: From E - V


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(6)    Judge whether we should freeze some modes.

0           read (*,*) label_frozen
                       0: Do not freeze any mode.
                       1: Freeze some modes
1 3         read (*,*) list_frozen
                       Give the list of the frozen mode.
                       The order of the normal mode number should be
                       same as the molden file.
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