peachgk_md Ver. 2.142 Input Script Manual (temporary)

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1. peachgk.ini

This script is most significant file in order to control peachgk_md. If you configure this file, you can utilize various functions implemented in peachgk_md as you want. In what follows, each parameter is explained precisely. The syntax of each line is

[parameter name] [value 1] [value 2] …

Since parameters other than the incorporated parameters are ignored by peachgk_md, you can insert any comment in the script. Inversely, if you delete the parameters present in the script, peachgk_md will cause malfunction. Therefore, even though you do not need a certain parameter or function, please leave that in the script.

The first line in the script shows the version information of peachgk.ini. If you change this line, peachgk_md is supposed to stop with error.

Frequently used parameters or significant parameters are presented in a **bold face** in what follows.

…peachgk.ini…

MD control script for peachgk Ver.5.6 '15.03.28

Configuration about input or output filenames

#input&output file name

iuwtopname	H2O_topOB.dat	Topology filename for water model (this file must be in the working directory.)
iuparavdwname	**para_vdw_s.dat**	Filename for the vdW (Lennard-Jones) parameter list (this file must be in the working directory.)
iuparabondname	**para_bond.dat**	Filename for the parameter list of bonded interaction parameters (this file must be in the working directory.)
iuparaconstname	para_const.dat	Filename for the pair list to which the rigid bond constraint is imposed (this file must be in the working directory.)
iuparacstmnbname	para_cstmnb.dat	Filename for parameters of a custom potential function (when using a custom

		potential function (ifcstmnb is ON), this file is needed.)
iuaddtopname	add_top.dat	Filename for parameters of additional topology information (needed when ifrdaddtop is ON)
iustrmvelname	out_strmvel.dat	Filename to input data of streaming velocity (ifstrmvel is ON)
iuposresname	sta_peachgk-2.0.dat	Filename for the reference coordinate data which is used to position restraint of atoms (ifposres is ON). The format of this file is the same as that of the following restart file.
iostarecname	**sta_peachgk-2.0.dat**	Restart filename of MD simulation
ousumname	out_sum.dat	Filename for summary of simulation conditions of a MD simulation
ouenename	**out_ene.dat .true.**	Filename for output energy data. A logical value of the last column indicates whether you actually want to output this file. (This is the case with the following items.)
ouposname	**out_pos.dat .true.**	Filename for output coordinate data of each atom
ouvelname	**out_vel.dat .true.**	Filename for output velocity data of each atom
outhename	out_the.dat .true.	Filename for output data regarding Nosé-Hoover thermostat
oubarname	out_bar.dat .true.	Filename for output data regarding barostat
ouprename	out_pre.dat .true.	Filename for output pressure data
outhcname	out_thc.dat	Filename for data regarding temperature control at local volumes when needed (ifoutthc is ON)
oupdbname	out_pdb.pdb	Filename for PDB formatted file when needed (ifoutpdb is ON)

Configuration about molecular species and number of molecules

#number of particle

In peachgk_md, all of the molecular species in the system are categorized into three types: polyatomic, water, and monatomic type. The program is designed so that it is much easier to do simulation when water and monatomic molecules are treated as the latter two types, respectively. Water can also be treated as the polyatomic type in principle if you want.

#number and type of each poly type
Format:
npolymoletyp No. npoly_mole npoly_atom iucorname iutopname createcor
!!! set the polytyp for createcor after the polytyp for rdstarec
!!! set "setcharge" to set partial charge value from cor file
!!! set "localfix" to fix the atom position (iflocalfix must be ON)
!!! set "localfixz" to fix the atom z position only (iflocalfixz must be ON)
Followed by index of atom to fix, and z position to fix.
!!! set "localfixzg" to fix the COM of molecule z position only
(iflocalfixzg must be ON) Followed by z position to fix.
!!! set "localheat" and the following real value to keep the temperature
to the target value (iflocalheat must be ON)
!!! set "posres" to impose position restraint (mole.) (ifposres must be ON)
!!! set "posresatm" to impose position restraint (atom) (ifposres must be ON)
Following the "posresatm", number of atoms for restraint,
indexes of atom for restraint are aligned.
Above posres schemes can be used with specifying the constraint
direction like posresx or posresatmy.
Do not use "posres" or "posresatm" together with direction-specifying
options like "posresx". "posres" means contraint for all directions.
!!! set "potbias" to impose the bias potential (mole.) (ifpotbias must be ON)
!!! set "potbiasatm" to impose the bias potential (atom) (ifpotbias must be ON)
Following the "potbiasatm", number of atoms exerted by the potential,
indexes of atom are aligned.
!!! set "pdbresname" and the following word (within 4 character)
to specify the "resname" in PDB format
!!! set "centerfix" to fix barycentric velocity of each molecular speices
(ifcenterfix_poly, _water, or _ma must be ON
and ifcenterfix_all must be OFF)

!!! set "localvel*" with the direction-specifying letter x, y, or z in '*'
or combinations of these options (localvelx and localvely, etc.)
followed by a velocity value (in m/s unit)
(iflocalvel must be .true. and centerfix of the atom must be .false.)

npolytyp 2 Number of polyatomic types in the system

npolymoletyp 1 5 24 C7H15OH_cor.dat C7H15OH_top.dat .true.

npolymoletyp 2 5 18 C5H11OH_cor.dat C5H11OH_top.dat .true.

↑These are the definition of molecular species and the number of molecules for each polyatomic type. In this example, there are two polyatomic types. From left to right, each column denotes [index (serial number)] [number of molecules] [number of atoms in a single molecule] [filename for molecular coordinate] [filename for molecular topology] [switch whether initial coordinates are generated] (these parameters are required). For other additional parameters, see comment lines above.

#npolymoletyp 3 5 18 C5H11OH_cor.dat C5H11OH_top.dat .true. setcharge pdbresname PENO

#npolymoletyp 4 5 18 C5H11OH_cor.dat C5H11OH_top.dat .true. localheat 300.0 posres pdbresname PENO

#npolymoletyp 4 5 18 C5H11OH_cor.dat C5H11OH_top.dat .true. localheat 300.0 posresx posresz pdbresname PENO

#npolymoletyp 5 5 56 C18H37S_cor.dat C18H37S_cor.dat .true. posresatm 1 1 pdbresname ODTI

#npolymoletyp 6 5 56 C18H37S_cor.dat C18H37S_cor.dat .true. localfixz 2 20.0e-10 pdbresname ODTI[

↑Some examples of description including additional parameters as comment lines

#number of water molecule

nwater 10 .true. Number of molecules for water type. The last column indicates whether initial coordinates are generated.

#number and type of each monatomic molecule
Format:
nmatomtyp No. nmatomtyp monoatmtyp createcor
!!! set the matyp for createcor after the matyp for rdstarec

nmatyp 2 Number of monatomic types

nmatomtyp 1 5 NA .true.

nmatomtyp 2 5 CL .true.

↑These are the definition of molecular species and the number of molecules for each monatomic type. In this example, there are two monatomic types. From left to right, each column denotes [index] [number of atoms] [identifier for molecular species with two letters] [switch whether initial coordinates are generated] (these parameters are required). For other additional parameters, see comment lines above.

#nmatomtyp 3 5 AU .true. localfix pdbresname GOLD

#nmatomtyp 4 5 PT .true. localheat 300.0 pdbresname PLAT

#nmatomtyp 5 1 FT .false. potbias pdbresname FE3P

#nmatomtyp 6 5 AU .true. localfixz 20.0e-10 pdbresname GOLD

↑Some examples of description including additional parameters as comment lines

#parameter of initial configuration for createcor

Format:

maxpo No. xmax ymax zmax and some other parameters

maxw No. xmax ymax zmax and some other parameters (No. = 1)

maxma No. xmax ymax zmax and some other parameters

Required parameters when initial coordinates are newly generated (coordinates are not restored from the restart file)

maxpo 1 1 1 5

maxpo 2 1 1 5

#maxpo 3 1 1 5 90.0

maxw 1 1 1 10

maxma 1 1 1 5

maxma 2 1 1 5

↑The index (series number) of second column corresponds to the index in the above block defining molecular species (nmatomtyp etc.) From left to right, each column indicates variables which is used in the creeatecor.F90 source code: [xmaxpo] [ymaxpo] [zmaxpo] (in the case of polyatomic type). In these parameters, the relationship of [xmaxpo]×[ymaxpo]×[zmaxpo] = [number of molecules in each species] must hold. Other additional parameters can be added and used in createcor.F90.

Configuration about MD ensemble and number of steps

#parameter of MD stages

mdcont_stage parameters

md_0k 0[K] NVT (clear distorsion)
md_h gradual heating NVT (v-scale)
md_t target temperature NVT (v-scale)
md_mtk NPT constant MD (MTK eq.)
md_nhc NVT constant MD (NHC eq.)
md_nve NVE constant MD
md_htf heat flux calculation in NVE MD (transflux.ini is needed)
md_ems energy minimization by steepest descent (SD) method

maxnstep **60000** Total number of MD steps

nstage **5** Total number of MD stages

↑In peachgk_md, total MD steps can be decomposed into multiple stages. The different ensemble or MD algorithm can be used in each stage, e.g., NVT in the first stage and NPT in the subsequent second stage. Summation of steps over all stages should be maxnstep above.

nstep_stage	**1**	**1000**	This line is linked to the next line. The second column is the series number.
mdcont_stage	**1**	**md_0k**	Perform temperature control MD at 0 K for 1000 steps (so-called quenched dynamics to relax the initial configuration).
nstep_stage	**2**	**29000**	
mdcont_stage	**2**	**md_t**	Perform constant temperature MD (velocity scaling) for 29000 steps.
nstep_stage	**3**	**10000**	
mdcont_stage	**3**	**md_mtk**	Perform NPT ensemble MD for 10000 steps using Martyna-Tobias-Klein equations of motion.
nstep_stage	**4**	**10000**	
mdcont_stage	**4**	**md_nhc**	Perform NVT ensemble MD for 10000 steps using Nosé-Hoover chain thermostat.
nstep_stage	**5**	**10000**	
mdcont_stage	**5**	**md_nve**	Perform NVE ensemble MD for 10000 steps.

↑See above comment lines for other available MD algorithms

nstep_maxwell -1 Time step for imposing Maxwell-

		Boltzmann velocity distribution. When -1 is used (non-existent time step), this algorithm is not used.
nstep_expand	-1	Time step for imposing expansion/shrink of computational cell size. When -1 is set, this algorithm is not used.

Configuration about MD system size

#cell dimensions (cel is prior to ratio)

xcel	**49.748536d-10**	Cell length in the *x* direction in [m] units
ycel	**49.748536d-10**	Cell length in the *y* direction in [m] units
zcel	**49.748536d-10**	Cell length in the *z* direction in [m] units
yratio	1.0d0	This gives ycel/xcel ratio. If ycel is not specified and this parameter is used, this ratio is employed to determine ycel.
zratio	1.0d0	This gives zcel/xcel ratio. If zcel is not specified and this parameter is used, this ratio is employed to determine zcel.
r_expand	1.1111111d0	Expansion/shrinkage ratio for the cell size when used (volume-based ratio).

Important parameters controlling MD simulation

#some important parameters

ifstarec	.false.	Restart MD simulation from the previous run written in the restart file.
ifcreatecor	.true.	Start MD simulation generating new coordinates of atoms. Code your initial configuration in createcor.F90.

↑You can choose both ifstarec and ifcreatecor at once. For example, this is conveniently adopted when coordinates of some parts of molecular species are given by the restart file, and the others are newly generated.

ifrdaddtop	.false.	Put additional topology information. The input script specified by iuaddtopname is

		required.
ifcenterfix_all	.true.	Keep the total translational momentum of the system zero (make modification every step). If this flag is ON, the following three parameters are ignored.
ifcenterfix_poly	.true.	Keep the translational momentum of polyatomic types zero individually.
ifcenterfix_water	.true.	Keep the translational momentum of the water type zero individually.
ifcenterfix_ma	.true.	Keep the translational momentum of monatomic types zero individually.

#PDB output

ifoutpdb	.true.	Output PDB formatted file.
nstep_pdbout	0	Using coordinates of this time step, PDB file is generated. Zero step means just before MD loop. So, this can be used to confirm initial configuration.

Configuration about MD time integration

#time step and MTS parameters

MTS flags

long-force long

med-force med ! Don't use this flag!

short-force short

In peachgk_md, the r-RESPA integration scheme is employed as a time integration. For multiple-time scale, the current version only support “long” and “short” timescales.

dt_long_cal	1.0d-15	Time step for long timescale integration in [sec] units
nstep_short	5	Number of inner loops for r-RESPA (short timescale). In this example, time step for short timescale integration is 1.0×10^{-15} / 5 = 0.2 [fs].

#!!! From Ver.1.74, do not use mts_med !!!

if you do not want to calculate certain interaction, just comment out,

then parallel computations become faster.

In the following configurations, specify which kind of interaction is calculated in which timescale (short or long). Note that if commented out, calculation of that interaction is skipped. When performing parallel computation, by commenting out unneeded interactions, the amount of inter-process communication can be reduced.

mts_bond	short	Bond stretching interaction
mts_angl	short	Angle bending interaction
mts_anglub	short	Urey-Bradley angle bending (CHARMM)
mts_tors	short	Torsion interaction (periodic type)
mts_torsrb	short	Torsion interaction (Ryckaert-Bellman type)
mts_torsim	short	Torsion interaction (improper)
mts_vdw	long	LJ potential
mts_ewr	long	Coulomb potential (real space)
mts_ewk	long	Coulomb potential (reciprocal space)
mts_vdw14	long	1-4 LJ potential
mts_elc14	long	1-4 Coulomb potential
#mts_mor	long	Morse potential
#mts_sh	long	Spohr & Heinzinger potential
#mts_rfh	short	Rustad, Felmy, and Hay potential
#mts_dou	long	Dou potential
#mts_cstmnb	long	Custom potential function
mts_cnpvw	long	Control of normal pressure by substrate wall
mts_posres	short	Position restraint force (harmonic bond)
mts_potbias	long	Bias potential

When making the initial configuration relaxed, the displacement of atoms is limited to a specified value in order to avoid the divergence of MD integration even if interatomic distances are extremely small.

iflimitmove	.false.	Limit the displacement of atomic motion
limitdist	0.1d-10	Maximum displacement of atoms in every time step in [m] units

Configuration about extended system MD

#Nose-Hoover chain and MTK eq. and higher order integration

for Nose-Hoover chain

mchain	3	Number of chains for the Nosé-Hoover chain method
tfreq	1.0d+13	Time constant for the Nosé-Hoover thermostat in [sec^{-1}] units
text	**300.0d0**	Target temperature in the Nosé-Hoover method in [K] units

↑If the time integration of Nosé-Hoover method is not stable, tweak the tfreq value. The above parameters are also adopted in the NPT simulation (md_mtk) as well as the NVT simulation (md_nhc).

for Andersen (Hoover type) barostat

vfreq	0.2d+12	Time constant for the barostat in the Andersen method in [sec^{-1}] units
pext	**0.1d6**	Target pressure in the Andersen method in [Pa] units
ifpatmcont	**.true.**	Pressure control by atom-based pressure
ifpmolcont	**.false.**	Pressure control by molecule-based pressure

↑Current version only supports the isotropic pressure control. If the pressure control integration is not stable, tweak the tfreq value. Either ifpatmcont or ifpmolcont must be enabled.

for higher order Trotter expansion

next	1	Repeating number of extended system using Trotter expansion
nyosh	3	Expansion order of Yoshida-Suzuki method compatible with 1, 3, and 5

↑In most cases, the default value is sufficient. Bigger values make the integration more accurate.

Other MD parameters

#some MD flags

ifrattle	.true.	Use SHAKE/RATTLE method
ifewald	**.false.**	Standard Ewald method for calculating Coulomb interaction

ifspme	**.true.**	SPME method for calculating Coulomb interaction
iffennell	**.false.**	Fennell (modified Wolf) method for calculating Coulomb interaction

↑One of above three parameters must be ON. However, if you enable FFLAGS2 = -D_LJ_ONLY in Makefile and compile peachgk_md (the system without partial charges), all three flags can be disabled. In this case, the calculation of the Ewald method is skipped and MD computation is made faster.

ifljari	.true.	Arithmetic mean is adopted to determine the LJ σ parameter between dislike atoms by default.
ifljgeo	.false.	Geometric mean is adopted to determine the LJ σ parameter between dislike atoms by default.

↑The mixing rule of σ parameter is controlled by A (arithmetic) or G (geometric) description in para_vdw_s.dat. However, for the atomic pair between A and G (not A-A and G-G pair), the above policy is employed for the mixing rule. All LJ ε parameters are evaluated by the geometric mean.

iflocalheat	**.false.**	Impose a temperature control by velocity scaling individually to each molecular species
ifregionheat	.false.	Impose velocity scaling to local volumes. The input script of tempcont.ini is needed in the working directory.
ifregionhf	.false.	Impose constant heat flux to local volumes (Jund & Jullien method). The input script of hfcont.ini is needed in the working directory.
ifreglange	.false.	Impose the Langevin thermostat to local volumes. The input script of langecont.ini is needed in the working directory.
iftcratom	**.true.**	When adopting the temperature control or heat flux control to local regions described above, the control is imposed to each atom (.T.) or each molecule (translational

		velocity of center of mass) (.F.). When the system has the molecules with rigid bond restraint, molecule-based control should be used. Otherwise, the rigid bond conditions would not be satisfied.
ifoutthc	.false.	When using temperature control to local volumes (velocity scaling and Langevin thermostat), the imposing and extracting thermal energy in one MD step is output to the file named by outthcname parameter
iflocalfix	.false.	Fix specific atomic or molecular coordinates (zero temperature)
iflocalfixz	.false.	Fix *z* coordinates of specific atoms or molecules
iflocalfixzg	.false.	Fix *z* coordinates of center of mass of specific atoms or molecules
ifposres	.false.	Constrain specific atomic or molecular coordinates using harmonic springs
ifpotbias	.false.	Apply the bias potential. The input script of potbias.ini is needed.
iflocalvel	.false.	Force to give the velocity to the specific atoms and molecules
ifstrmvel	.false.	Input the streaming velocity from the external file and calculate proper temperature and heat flux when the streaming velocity exists. This file can be generated by post-process code of process_data/lvs_vel/. The file name is determined by the iustrmvelname parameter.

↑Most of the above parameter work with the parameters in the "#number of particle" block mentioned above (configurations for molecular species and the number of molecules).

#!!! if you use NPT dynamics, you must choose ifcalpremole or ifcalpreatom !!!

ifcalpremole	**.true.**	Calculate molecular pressure

ifcalpreatom	**.true.**	Calculate atomic pressure
ifnetqcorrp	.true.	If the system has net charge, the correction to the pressure values is evaluated.

↑When using the pressure control (md_mtk), the corresponding pressure calculation should be performed.

pressure calculation of L-J long-range correction

ifcalljlong	.false.	Employ the long range correction to the pressure associated with LJ cut-off. Since this algorithm can be used in the quite limited situations (water system), see what is done in the code.
solvetyp	OB	Identifier of the target oxygen atom to which the long range correction is adopted
nsolve	10	Number of solvent molecules

parameter for ewald method

alpha	**2.9202899d9**	α parameter in the Ewald method in [m^{-1}] units
kmax	8	Extension of reciprocal space in the standard Ewald method
rrcut	**9.0d-10**	Cut-off radius for the real space calculation in the Ewald method in [m] units

parameter for SPME method

#!!! FFT requires grid points are a multiple of 2,3,5

nfft1	**50**	Number of charge grids in the *x* direction in the SPME method
nfft2	**50**	Number of charge grids in the *y* direction in the SPME method
nfft3	**50**	Number of charge grids in the *z* direction in the SPME method
pme_order	6	Order of B-spline function in the SPME method

↑The charge grid spacing should be almost 1Å adjusting the number of charge grids.

parameter for energy minimazation

d_rini	0.5d-10	Initial displacement of atoms in the energy minimization using the steepest descend method in [m] units
d_rmax	1.0d-10	Maximum displacement of atoms in the energy minimization using the steepest descend method in [m] units
d_econv	1.0d-24	Convergence error of energy in the energy minimization using the steepest descend method in [J] units
d_rmsf	1.0d-13	Convergence error of root mean square force in the energy minimization using the steepest descend method in [N] units

other MD parameters

rcut	**12.0d-10**	Cut-off radius for LJ interaction in [m] units
ifcellindex	**.true.**	Use cell-index method
ifbook	**.true.**	Use book-keeping (neighbor list) method
rcut_book	**14.0d-10**	Cut-off radius for the book-keeping method in [m] units. This value must be larger than rcut and rrcut.
nstep_book	**50**	Update the neighbor list every what time steps

↑If there is no particular reason, both ifbook and ifcellindex should be ON. When the system size is not enough to employ the cell-index method, the cell-index is turned off. rcut_book and nstep_book parameters should be properly determined by users, checking NVE simulation, for example.

tcont_poly	**300.0d0**	Target temperature for the velocity scaling method in [K] units (polyatomic type)
tcont_water	**300.0d0**	Target temperature for the velocity scaling method in [K] units (water type)
tcont_ma	**300.0d0**	Target temperature for the velocity scaling

		method in [K] units (monatomic type)
tcont_poly_ini	**0.0d0**	Initial temperature for the gradual heating/cooling scheme (md_h) in [K] units (polyatomic type)
tcont_water_ini	**0.0d0**	Initial temperature for the gradual heating/cooling scheme (md_h) in [K] units (water type)
tcont_ma_ini	**0.0d0**	Initial temperature for the gradual heating/cooling scheme (md_h) in [K] units (monatomic type)

↑When iflocalheat is disabled, tcont_poly is representative to the target temperature of the system. When doing a md_h simulation, starting from initial temperature of tcont_*_ini, the system temperature is gradually increased/decreased up to the final temperature of tcont_* in the corresponding number of MD steps.

tcontinterval	**100**	Impose velocity scaling every this time steps
outinterval	**100**	Output various data every this time steps
pressinterval	**100**	Output pressure data every this time steps
heatfinterval	100	Output heat and momentum flux data every this time steps
recinterval	**1000**	Output restart data every this time steps. The restart file is overwritten. In addition, the restart file is overwritten at the end of the MD simulation.
oatmtyp	OB	Identifier for oxygen atom of water type (The default is SPC/E model)
hatmtyp	HB	Identifier for hydrogen atom of water type
randseed	555	Random seed
compfact	1.00d0	Parameter for the initial configuration
eps_rattle	1.0e-7	Convergence condition for the SHAKE/ RATTLE method

#Spline interpolation for ewald real space calculation

nspltbl	**1100**	Number of samples for the table-based interpolation applied to the complementary error function used in the Ewald method

↑The larger number of samples makes the interpolation more accurate, while it makes the computational cost larger in association with the latency of memory access. It is desirable that each user optimizes this parameter in their system. The recommended value is estimated by (rrcut [Å] + 2) * 100 and in most cases, this leads to the sufficiently accurate potential energy.

Configurations about cut-off radius for each interaction function

Cufoff setting for special interaction functions

#Morse cutoff

rcutmor	12.0d-10	Cut-off radius for Morse potential in [m] units
ifcellindex_mor	.false.	Use cell-index method for Morse potential
ifbookmor	.false.	Use book-keeping (neighbor list) method for Morse potential
rcut_bookmor	14.0d-10	Cut-off radius of the book-keeping method for Morse potential in [m] units
nstep_bookmor	50	Update the neighbor list for Morse potential every what time steps

In what follows, the similar configurations for each interaction function are repeated.

:

:

#RP-VW cutoff

Configuration regarding the normal pressure control using virtual walls (the detailed algorithm is omitted)

ifcnp	.false.	Use the normal pressure control by virtual walls
rcutrpvw	12.0d-10	Cut-off radius for the interaction between the virtual wall and the real system in [m]

		units
#ifcellindex_rpvw	.false.	! **dummy** flag for cell index (RP-VW)
ifbookrpvw	.false.	Use the book-keeping (neighbor list) method for the interaction between the virtual wall and the real system
rcut_bookrpvw	14.0d-10	Cut-off radius of the book-keeping method for the virtual wall interfaction in [m] units
nstep_bookrpvw	50	Update the neighbor list for the virtual wall interaction every what time steps

Configuration regarding a custom potential function

#CUSTOM NB interaction flags

ifcstmnb	.false.	Use a custom potential function
ifcellindex_cstmnb	.false.	Use the cell-index method
ifbookcstmnb	.false.	Use the book-keeping (neighbor list) method

↑Other detailed parameters are defined in the para_cstmnb.dat file in the corresponding directory of the custom potential function.

END

…peachgk.ini until here…

2. Input files for molecular models

2.1. para_bond.dat

2.2. para_vdw_s.dat

2.3. para_const.dat

2.4. Molecular topology file (*_top.dat)

2.5. Molecular coordinate file (*_cor.dat)

To be updated