

Chapter 4 CONFLEX Keyword Options

In order to run a conformational search or a crystal structure search using CONFLEX, an initial settings file (.ini) containing the keywords for the settings must be created beforehand. When there is no .ini file, structural optimization using the default MMFF94s force field is carried out.

When calculations are run from the CONFLEX Interface, an .ini file is generated automatically.

The .ini file can be created using a text editor. Keywords (switches) and their descriptions are listed below.

Please note: If multiple options are designated for a keyword which requires only one option, inaccurate results may be generated.

Force Field Settings

Keyword	Options	Description
EMM2		Extended MM2 force field is used for calculation.
MM2		MM2 force field is used for calculation.
MM3		MM3(92) force field is used for calculation.
MMFF MMFF94		MMFF94 force field is used for calculation.
MMFF94S		MMFF94s force field is used for calculation.(Default)
DIELEC=	f,ff	Definition of the dielectric constant of the force field calculation employed. By default, this value is set to 1.0 for MMFF and 1.5 for MM2 and MM3.
ELECSTAT=	BCI NQE BOND_DIPOLE	The method of electrostatic calculation is changed. Although the electrostatic term is inherent in the force field (BCI for MMFF94 and MMFF94s, etc), user can select the other methods for the calculation.
PSEUDO_BOND= PSEUDO_DIST=	(I,J,STD,FK)	Pseudo force between I-th and J-th atoms is provided. When standard length STD and force constants FK of harmonic potential function are set to zero, the distance (angs.) of the initial structure and 10,000 (kcal/mol/An ^{gs} ²), respectively are given as the defaults.
PSEUDO_ANGL=	(I,J,K,STD,FK)	Pseudo force of I-J-K angle is provided. When standard angle STD and force constants FK of harmonic potential function are set to zero, the angle (deg) of the initial structure and 10,000 (kcal/mol/rad ²), respectively are given as the defaults.
PSEUDO_TORS=	(I,J,K,L,STD,FK)	Pseudo force of I-J-K-L torsion angle is provided. When standard angle STD and force constants FK of harmonic potential function are set to zero, the angle (deg) of the initial structure and 1,000 (kcal/mol/rad ²), respectively are given as the defaults.
PSEUDO_OOPL=	(I,J,K,L,STD,FK)	Pseudo force of I=J-K(-L) out-of-plane angle is provided. When standard angle STD and force constants FK of harmonic potential function are set to zero, the angle (deg) of the initial structure and 1,000 (kcal/mol/rad ²), respectively are given as the defaults
PSEUDO_PHI5=	(I,J,K,L,M,STD,FK)	Pseudo force of 5-membered ring phase angle is provided. When standard angle STD and force constants FK of harmonic potential function are set to zero, the angle (deg) of the initial structure and 1,000 (kcal/mol/rad ²), respectively are given as the defaults.
PSEUDO_HALF=	(I,J,STD,FK)	Pseudo force of elongation between I-th and J-th atoms is provided. When standard distance STD and force constants FK of half harmonic potential function are set to zero, the angle (deg) of the initial structure and 1,000 (kcal/mol/rad ²), respectively are given as the defaults.

Keyword	Options	Description
PSEUDO_MORS=	(I,J,STD,FK,ALFA)	Pseudo force with Morse function is provided. When standard distance STD and force constants (dissociation energy) FK and direction factor ALFA are set to zero, the distance (angs.) of the initial structure, 1,000 (kcal/mol/rad ²), and +1.0 (kcal/mol), respectively, are given as the defaults.
SET_VELEC=	(I,J)	Temporary change the hybridization of the I-th atom into J value. Where I is a serial number of the atom that will be changed the number of valence electrons by user, and J is the number of valence electrons of the I-the atom.

Geometry Optimization Keywords

Keyword	Options	Description
OPT= Default : full-matrix Newton-Raphson Method (NEWTON) Example : OPT=CONGRD		Geometry optimization method
	STEEPD	steepest descent method
	CONGRD	conjugate gradient method
	VARMET	variable metric method
	NEWTON	full-matrix Newton-Raphson method
	NONE	In the case of "OPT=NONE", only energy calculation will be performed for the input structure.
	FAST	"FAST" is a special setting for large molecule. This is corresponding to the following keywords: "OPT=CONGRD TG=1.0 GCONV_CG=1.0D-3 XCONV_CG=1.0D-4"
	PRECISE	"PRECISE" is a sequential procedure of STEEPD, CONGRD, and NEWTON. When this option is selected, some convergence criterion set to the following values: "TG=1.0 GCONV_CG=1.0D-3 XCONV_CG=1.0D-4 GCONV_NR=1.0D-6 XCONV_NR=1.0D-6"
IRC_FMF=	n	FMF method follows the n-th eigen vector. Default is "1", which means the first eigen vector will be follows to search for the corresponding transition state.
NOOPT		Only energy calculation will be performed for the input structure. This keyword corresponds to "OPT=NONE".
OPTBY= Example : OPTBY=GRADIENT	ENERGY GRADIENT	Objective function to be minimized during geometry optimization. Default is ENERGY.
TG= Example : TG=2.5	ff.ff	Gradient threshold for pre-optimization (steepest decent Method). By default TG is set to 5.0 kcal/mol/Angs.
GCNVRG= Example : GCNVRG=1.0E-5	ff.ff	Threshold of gradient convergence for geometry optimization. By default GCNVRG is set to 1.0E-6 kcal/mol/Angs.
XCNVRG= Example : XCNVRG=1.0E-5	ff.ff	Threshold of atom displacement convergence for geometry optimization. By default XCNVRG is set to 1.0E-6 kcal/mol/Angs.

Keyword	Options	Description
STEEPD= CONGRD= VARMET= NEWTON=	(Gconverg,Xconverg)	Threshold of energy gradient (Gconverg) and atom displacement (Xconverg) convergence for geometry optimization by using each method.
MAXITR_SD= MAXITR_CG= MAXITR_VM= MAXITR_NR=	n	Maximum number of iterations for geometry optimization. _SD for steepest decent, _CG for conjugated gradient, _VM for variable metric, and _NR for Newton-Raphson method.

CONFLEX Conformation search keywords

Keyword	Options	Description
CONFLEX		Conformation search will be performed.
SEL=	ff.ff	The value of "SEL" defines the search limit that controls the range from which the initial structures are selected. If the value of "SEARCH" is "ENERGY", the search limit is defined in kcal/mol, and if "BOLTZ", the search limit is defined in % population according to Boltzmann distribution. By default, this value is set to 10 kcal/mol, namely, the corresponding keywords as follows: Example : SEL=10.oDo SEARCH=ENERGY See also "SEARCH="
SEARCH= Example : SEARCH=ENERGY	ENERGY BOLTZ	Definition of the evaluation unit for the search limit. If the value of "SEARCH=" is "ENERGY", the search limit is defined in kcal/mol, and if "BOLTZ", the search limit is defined in % population according to Boltzmann distribution. By default, this value is set to ENERGY. See also "SEL=".
MAXINIT= MAXSTACK= Example : MAXINIT=4	n	Number of the initial structures used for a generating process of trial structures.
MAXCYCLE= Example : MAXCYCLE=1	n	Number of search cycles is fixed. In general, the number of search cycles can not defined by user, because of SEL value control (see "SEL="). This keyword, that forcibly sets the limit of search cycles, should be used only for evaluating an time-consuming of the practical conformation search.
ADD_CONFIG_RS=	l	Tetrahedral configuration around the l-th centre atom can be fixed during CONFLEX search, even if the l-th atom is not chiral center of atom.
ADD_CONFIG_EZ=	(l,J,K,L)	Torsional configuration defined by l-J-K-L dihedral angle can be fixed during CONFLEX search, even if the J-K bond is not double bond.
FLAP		If the corner-flapping perturbation is possible, it will be performed.
NOFLAP		The corner-flapping perturbation is prohibited, even if it is possible.
FLAP_SELECT=	l	User can specify a flapping atom as the l-th atom. When this option is used, flapping atom list, which is automatically determined, must be ignored.
FLAP_DESELECT=	l	User can remove the l-th atom from the flapping atom list, which is automatically determined. The specified l-th atom is prohibited from flapping perturbation.
FLIP		If the edge-flipping perturbation is possible, it will be performed.
NOFLIP		The edge-flipping perturbation is prohibited, even if it is possible.
FLIP_SELECT=	(l,J)	User can specify a flipping bond between the l-th and J-th atoms. When this option is used, flipping bond list, which is automatically determined, must be ignored.

Keyword	Options	Description
FLIP_DESELECT=	(I,J)	User can remove the I-J bond from the flipping bond list, which is automatically determined. The specified I-J bond is prohibited from flipping perturbation.
SROT		If the stepwise rotation perturbation is possible, it will be performed.
FIXED_SROT_NSTEP=	n	Number of rotational isomers expected in stepwise rotation for a bond is fixed to n. (n-1) trial structures will be generated from each of the initial structures.
NOSROT		The stepwise rotation perturbation is prohibited, even if it is possible.
SROT_SELECT=	(I,J,N)	User can specify a stepwise rotatable bond between the I-th and J-th atoms. When this option is used, SROT torsional bond list, which is automatically determined, must be ignored.
SROT_DESELECT=	(I,J)	User can remove the central I-J bond from the SROT torsional bond list, which is automatically determined. The specified I-J bond is prohibited from stepwise rotational perturbation.
XSROT_PEPTIDE_BOND		All peptide bonds (CO-NH) of the molecule are removed from SROT list, and their s-cis/trans stereo-configurations will be kept the initial situation during CONFLEX search.
CHECK=		This keyword defines the conformational similarity indices. In conformational space search, the program must check the conformation redundancy of the newly optimized structures with the already-known structures stored in conformation database. In CONFLEX, the potential energy values are always used in this purpose, because the severe full-matrix Newton optimization can reach to 1.0D-6 kcal/mol/Angs. In scarce cases, however, the energy does not work enough for the correct distinction of conformation. That is why the following similarity indices are prepared for the additional comparison between two conformers:
Example : CHECK=(XCORD,HEAVY)		
	XCORD	XCORD: the difference of the molecular atomic coordinates that are reoriented to a standard orientation based on the moment of inertia is directly compared.
	TORSION	TORSION: the sum of Root-mean-square differences in the corresponding pair of torsion angles of skeleton bonds is compared.
	MOMENT	MOMENT: the difference of the axis components in the moment of inertia is compared.
	NOENERGY	NOENERGY: those additional comparisons without the potential energy comparison are performed. Otherwise, the energy check is always performed.
	HEAVY	HEAVY: positions of all hydrogens will be ignored in XCORD comparison.
ESAV=	ff.ff	Defines the highest potential energy (EGYMAX) of the stored conformer: EGYMAX = ESAV + the potential energy of the global energy-minimum conformer (GEM). By default, ESAV is set to N/2 kcal/mol (N = total number of atoms in the molecule). Those conformers having the relative potential energies smaller than ESAV from the GEM, are stored into the conformation database, but those having potential energy higher than EGYMAX are discarded. The efficiency and the reliability of CONFLEX search is greatly influenced by the number of stored structures. A small ESAV leads to a smaller number of stored structures and less computer time, but the risk of missing significant conformers increases. This is because unstable conformers sometimes produce stable conformers upon local perturbation. On the other hand, a large ESAV ensures finding all significant conformers but leads to longer calculation time.
Example : ESAV=6.5		
EDIF_HARD=	ff.ff	Threshold of the basic comparison in potential energies if "CHECK=NOENERGY" is not specified. See also "CHECK=".
Example : EDIF_HARD=1.0D-5		
EDIF_LOOSE=	ff.ff	Threshold for the comparison of potential energies in the first stage of redundancy test when "CHECK=TORSION" is specified. If a new conformer has the same potential energy, within this range, with one of the stored structures, the program proceeds to the torsion angles test. The default is 3N/100 kcal/mol.
Example : EDIF_LOOSE=2.0		

Keyword	Options	Description
GRMS_HARD= Example : GRMS_HARD=1.0D-5	ff.ff	One of the thresholds in the RMS average of the final gradient for the termination of the geometry optimization.
GRMS_LOOSE Example : GRMS_LOOSE=1.0D-7	ff.ff	One of the thresholds for the RMS average of the final gradient for the termination of the geometry optimization.
XCOD_MAX= Example : XCOD_MAX=1.0	ff.ff	One of the thresholds in the maximum displacement of each optimized step during the iterative geometry optimization.
XCOD_RMS= Example : XCOD_RMS=4.0	ff.ff	One of the thresholds in the RMS averaged displacement of each optimization step during the geometry optimization.
TORS_MAX Example : TORS_MAX=1.0D-2	ff.ff	Threshold of the comparison in the maximum difference in torsion angles if "CHECK=TORSION" is specified.
TORS_RMS Example: TORS_TMS=1.0D-1	ff.ff	Threshold of the comparison in the RMS average of difference in torsion angles if "CHECK=TORSION" is specified.
MOMT_MAX Example : MOMT_MAX=0.5	ff.ff	Threshold of the comparison in the maximum difference in the components of the moment of inertia for the optimized structure if "CHECK=MOMENT" is specified.
MOMT_RMS Example : MOMT_RMS=0.1	ff.ff	Threshold of the comparison in the RMS average of difference in the components of the moment of inertia for the optimized structure if "CHECK=MOMENT" is specified.

Molecular Object Group Option

Keyword	Options	Description
MOL_GROUP=	(i,n)	Molecular object group that is containing a molecule or a few molecules in a molecular complex system (consisting of some molecules) will be defined. For example, description of "MOL_GROUP=(3,1)" in the ini-file means all atoms of one molecule having No. 3 atom (i=3) will be classified to the first (No. 1) molecular object group (n=1) automatically. If some molecules are collected together with one molecular object group, this option can be used repeatedly.
GOPT=	CONGRD NEWTON	Optimization method of the target molecular object group specified by "MOL_GROUP=" can be selected. "GOPT" without specification corresponds to "GOPT=(CONGRD,NEWTON)". Optimization method of the target molecular object group specified by "MOL_GROUP=" can be selected. "GOPT" without specification corresponds to "GOPT=(CONGRD,NEWTON)".
GOPT_HYDROGENS		All hydrogens are are classified and subject to optimization before optimizing the target molecular object group.
GOPT_SCF_CYCLE=	n	Maximum number of SCF cycles of molecular group optimization. Default is equal to 1.
GOPT_ECNRG=	f.f	Energy threshold (kcal/mol) for SCF cycles of molecular group optimization. Default value is equal to 1.0D-4

Vibrational Analysis Keywords

Keyword	Options	Description
THERMO= Example : THERMO=XYZ	XYZ INTER HEVYLP	Vibrational analysis, that is equivalent to the normal mode analysis using the mass weighted second derivative matrix, will be performed if the structure enough to be optimized is given. Thermodynamics functions, the vibrational frequencies and the corresponding mass weighted vibrational modes are also printed. "XYZ" and "INTER" control the printing form in Cartesian and internal coordinate system, respectively. The default is "XYZ". If "HEVYLP" is specified, lone pairs are packed into the elements of the second derivative matrix at the attached heavy atom.
NOTHERMO		Does not perform any thermodynamic calculation and also print out any vibrational mode or eigenvectors.
EIGVEC= Example : EIGVEC=XYZ	XYZ INTER HEVYLP	Normal mode analysis without the mass weighted second derivative matrix will be performed, and then eigen values and eigen modes are written to the output file. "XYZ" and "INTER" control whether the information is written to the output file as Cartesian or Internal coordinate formats, respectively. If "HEVYLP" is specified, lone pairs are packed into the elements of the second derivative matrix at the attached heavy atom. Default is "XYZ".
TEMP= Example : TEMP=30.0	ff.ff	Temperature is specified to ff.ff degrees centigrade (°C); by default it is set to 25.0
ALLMODE		Print out all vibrational modes computed.
LOWMODE=	ff.ff	Print out vibrational modes or eigenvectors less than n th of them.
NOMODE		Thermodynamic calculation will be performed, but never been printed any vibrational mode or eigenvectors.
PROJECT_OUT= Example : PROJECT_OUT=6	n	In normal mode analysis of single non-linear molecule, although six degrees of freedom corresponding to three translation and three rotational motions must be presented as near-zero vibrational frequencies (very very small vaules in wave number unit), it is very difficult to reach in the practical computation of a complicated molecule. To reduce any unexpected effect of those non-zero vibrational motions, this option can project out some components of non-zero vibrational modes lower than n-th vibrational frequency's mode from the Hessian second derivative matrix.

PDB File loading options

Keyword	Options	Description
PDB_MUTATE=	(resname,chain,num)	<p>One amino residue having chain of chain ID and num of residue number described in PDB file can be replaced to a standard amino residue specified by resname of the amino residue. Elongation of the sidechain will be automatically folded by minimizing the following evaluation function:</p> $f = \begin{cases} \sum_i \frac{k}{2} (r_i - R)^2 & (R > r_i) \\ 0 & (R \leq r_i) \end{cases}$ <p>where r_i is a non-bonded distance between an elongated atom i and the other atom, R and k are the considerable distance threshold and the force constant, respectively. Name of amino residues for resname can be described by using any type of three nomenclatures: one character (A, N, C, E, H, etc.), three characters (ALA, ASN, CYS, GLU, HIS, etc.), and full-name of amino acid (alanine, asparagine, cysteine, gulutamic_acid, histidine, etc.).</p>
PDB_NOMUTATE		Missing atoms of amino residue are not added. Therefore, "PDB_MUTATE=" option must be required for the correct application of computational chemistry to peptides and proteins.

PDB_THRESH=	R	Distance threshold in angstrom.
PDB_KCONST=	k	Force constant in kcal/mol/Angs ² .
PDB_HETATM		All atoms in "HETATM" records are considered for calculation. (default)
PDB_NOHETATM		All atoms in "HETATM" records are ignored.
PDB_WATER		"HOH" atoms in "HETATM" records are used for calculation. (default)
PDB_NOWATER		"HOH" atoms in "HETATM" records are ignored.
PDB_MODEL_NO=	n	Selection of the model serial number that specifies an ensemble to. Default is the first model that is corresponding to "PDB_MODEL_NO=1". If no entry of "MODEL" record in the PDB file, all atoms are used for calculation.
PDB_SSBOND		Connect the S-S bonds that are specified in "SSBOND" record.
PDB_NOSSBOND		All "SSBOND" records are ignored.
PDB_SSB_DIST=	ff.f	Distance threshold of S-S bond connection
PDB_CONECT=	(I,J,K)	Bonding between I and J atoms with K-bond type K=1: SINGLE K=2: DOUBL K=3: TRIPLE K=4: IONIC(I+,J-)
PDB_DISCONNECT=	(I,J)	A bond between I and J atoms is forcibly disconnected.
PDB_CHARGE=	(I,K)	Put a formal charge K on I atom. For example, when you explicitly specify that a calcium ion with atom No.1354 has +2 formal charge, keyword description is "PDB_CHARGE=(1354,+2)".

Conformation Clustering Keyword

Keyword	Options	Description
CLUSTER		Conformation clustering will be performed by using a single linkage algorithm. This keyword should be used with "CONFLEX" keyword.
CCLUS_DISTANCE=		Definition of conformation distance (similarity) to be used for conformation clustering.
	TORSION	rms difference of torsion angles
	ATOM	rms difference of atomic position after super-imposing
CCLUS_REFALL=		Automatically defines the reference atoms or torsion angles to determine the conformation distance. When "TORSION" is selected to the conformation distance ("CCLUS_DISTANCE="), the following options can be specified:
	TORSION	all torsion angles to be used for energy calculation
	COMPAR	all torsion angles to be used for comparison with conformers
	PHIPSI	all phi/psi torsion angles of peptide (PHIPSI) (only for peptide)
		When "ATOM" is selected to the conformation distance ("CCLUS_DISTANCE="), the following options can be specified:
	ALPHA	all alpha carbons of peptide (only for peptide)
	HEAVY	all heavy atoms
NOHYD	all atoms except for hydrogen	
CCLUS_IREF=	I (I,J)	The atom number of the referenced atom, or atom numbers of the central bond of the reference torsion angle. This keyword uses one line to specify one reference.
CCLUS_XREF=	I (I,J)	The atom number of the atom to be excluded from reference atoms, the atom numbers of the central bond to be excluded from reference torsion angles. This keyword uses one line to specify one reference.

Keyword	Options	Description
CCLUS_LIMIT=	f.ff AUTO	Threshold of conformation clustering automatically prepares the threshold of conformation distance (AUTO)
CCLUS_LIMIT_MAX=	f.ff	Threshold of for constraint clustering
CCLUS_EGFUNC=		Sort index is specified.
	STERIC	sorted by the "STERIC" energy order
	FREE	sorted by the Gibbs "FREE" energy order
CCLUS_MAXCONF=	n	Maximum number of conformers referenced in conformation clustering.

UV/Vis/CD Spectrum and PPP/SCF-MO keyword

Keyword	Options	Description
UVCD		UV/Vis/CD Spectrum calculation will be performed.
CDUV		Same with "UVCD"
PIA_OPT=		In PPP/SCF-MO calculation, all PI-atoms are automatically selected. However, SCF Instability is often caused by including some types of PI-atoms, carbonyl and peptide bonds in widely distributed aromatic system.
	NOPEP	NOPEP: excluding all peptide bonds (CONH)
	NOATE	NOATE: excluding all carboxyl groups (COO)
PIA_DEL=	I	Excluding I atom from PI-atoms
SCF=		Selection of SCF methods
	PPP	PPP: General PPP/SCF-MO calculation
	VESCF	VESCF: Variable electronegativity calculation (Allinger's approach)
PPP=		Extensions of SCF-PPP calculation.
	VB	Variable beta method
Example : PPP=(VB,VG)	VG	Variable gamma method
	NEWG	New gamma method
SCF_ITER=	N	Maximum number of SCF iterations.
SCF_CONV=	f.ff	Threshold of SCF convergence.
CIS= Example: CIS=(10,10)	(Nomo,Numo)	Specifies the number of electrons on the occupied and unoccupied molecular orbitals considered in Single-CI calculation.
CURVE_PLOT=	(f1,f2,f3)	Range of spectrum, and incremental width for curve-fitting based on the gauss approximation. f1: Starting point in wave number (cm ⁻¹) f2: Terminal point in wave number (cm ⁻¹) f3: Incremental step width in wave number (cm ⁻¹) Default: CURVE_PLOT=(10000.0,70000.0,200.0) In this case, the spectrum values at total 301 points are reported.
CURVE_DSIGMA=	f.ff	Standard deviation of the Gaussian distribution. Default value is 2000.0 cm ⁻¹

Solvent Effect Analysis Related Keywords using Generalized Born (GB/SA)

Keyword	Options	Description
GBSA		GB/SA calculation will be performed.
GBSA_ANALYZER= Example: GBSA_ANALYZER=FREE	SINGLE OPTIMZ FREE	Solvation energy analysis based on GB/SA calculation will be performed. In all options, GB/SA calculation will be performed after geometry optimization in gas phase. These options are set to the type of GB/SA calculation: -single-point (SINGLE) -geometry optimization (OPTIMZ or FREE) Solvation energy is defined by the total energy difference between gas phase and in solvent (SINGLE and OPTIMZ) or defined by the free energy difference between gas phase and in solvent (FREE).
GBSA_SOLVENT=	WATER OCTANOL	Solvent type is specified. If no solvent name, water environment will be applied as default, but octanol parameter is unavailable yet.
MOL_DIELEC=	f.ff	Definition of the dielectric constant of molecule. By default, this value is set to 1.0.
SA=	NUM	The calculation of solvent accessible surface area will be performed numerically.
NLR=	ON OFF	Neighbor-List Reduction will be performed. By default, this value is set to ON.
INIT_GEOM=	SAME	Initial geometry for the calculation that is including solvent effect is set to same as input geometry.

For the calculation including GB/SA solvent effect, it is necessary to have two types of parameters: one is for LCPO method, and another is surface tension coefficient.

The parameters of the LCPO method used to estimate the surface area are provided with the following MMFF atom type number:

1-3, 5-12, 15, 21, 23, 24, 27-29, 32, 34, 36-41, 44, 54-57, 59, 63-66, 71, 78

The surface tension coefficient parameters used to estimate the non-electrostatic energy multiplied by the surface area are provided with the following MMFF atom type number:

1-3, 5-8, 10-12, 15, 21, 23, 24, 28, 29, 37, 71

Please see the following papers for force field and type of atom

Thomas A. Halgren, J. Comput. Chem., 17, 490-519 (1996).

Crystal Structure Optimization keyword

Keyword	Options	Description
CRYSTAL		Crystal calculation will be performed.
SPACE_GROUP=	P1 P21 P212121 etc...	Definition of the Hermann-Mauguin space group symbol can be selected. Descriptions of the options are shown in APPENDIX.
SPGP_SUBINFO=		Monoclinic SPGP settings; Default is 'B'.
	B	Monoclinic cell with the B unique axis ($\alpha, \gamma = 90.0^\circ$).
	C	Monoclinic cell with the C unique axis ($\alpha, \beta = 90.0^\circ$).
		Origin setting; Default is '1'.
	1	origin choice 1
	2	origin choice 2
		Trigonal SPGP setting; Default is 'H'.
	R	Trigonal using rhombohedral axes ($a=b=c, \alpha=\beta=\gamma \neq 90^\circ, <120^\circ$)
	H	Trigonal using hexagonal axes ($a=b \neq c, \alpha=\beta=90^\circ, \gamma=120^\circ$)
LATTICE_CONSTANT=	(a,b,c, α,β,γ)	Definition of lattice constants
CRYSTAL_OPTIMIZATION=		Crystal optimization setting.
Default : CRYSTAL_OPTIMIZATION=RIGID	MOL	Referenced molecular structure will be optimized.
	RIGID	Lattice constants, molecular orientation (Euler angles of the molecular rotation), and molecular translation will be optimized.
	ALL	Referenced molecular structure, lattice constants, molecular orientation, and molecular translation will be optimized.
	NONE	Crystal structure optimization will be not performed.
CRYSTAL_RADIUS=	f.ff	Radius of nanoscopic spherical crystal can be specified. Default value is equal to 20.0 angstroms. To apply the consistency constraint for MPI parallel computations, this keyword will be designated. Unfortunately, this keyword requires a proportionate amount of the MPI-master computer's memory depending on the number of atoms in the crystal and of MPI-workers.
CRYSTAL_RESETUP_CONVERGE=	ff.ff	This keyword controls the reconstruction of the crystal structure in optimization. In each optimization step, if the RMS average of the energy gradients is less than the specified threshold (ff.ff kcal/mol/angstroms.), the reconstruction of the crystal structure before the next iteration is skipped. Unstable convergence of the crystal structure optimization is sometimes caused by the change of the number of the crystal constituent molecules with the reconstruction. Therefore, adjustment of the threshold may need to avoid the obstacle.
Default: 1.0E-3		
SUPERCELL=	(l,m,n)	Create supercell. The supercell is defined by basis lattice vectors, A, B, C, which are respectively represented by integral multiples of basis lattice vectors, a, b, c, of original unit cell, i.e. $A=la, B=mb, C=nc$. And the supercell naturally has P1 symmetry. For example, in the case of "(2,2,1)", the supercell are composed of one original unit cell and three replica unit cells which are generated by translating original unit cell along a axis and b axis.
MAKEP1CELL		Create a unit cell which has P1 symmetry. This keyword is corresponding to "SUPERCELL=(1,1,1)". See above.

Keyword	Options	Description
CIF_BOND= Example: CIF_BOND=(1,2,2)	(I,J,K)	Bonding between I and J atoms with K-bond type for using CIF file. K=1: Single K=2: Double K=3: Triple
CIF_FCHARGE= Example: CIF_FCHARGE=(1,-1)	(I,K)	Put a formal charge K on I atom for using CIF file.
BOND_LENGTH=	(m,I,J,ff.ff)	Modification of bond length. When m=0, I and J indicate serial number in model. Atom J position is adjusted along vector from atom I to atom J, and bond length between I and J atoms is converted to ff.ff. When m=1, I and J are atomic number. Atomic number J positions are adjusted along vector from atomic number I to atomic number J, and all bond lengths between defined atomic elements are converted to ff.ff. For example, in the case of "(1,8,1,0.983)", all bond length between hydrogen atom and oxygen atom are converted to ff.ff by adjusting hydrogen atom positions.
HYGEN_LENGTH		All lengths of bond which have covalently attached hydrogen atom are converted to equivalent bond lengths in using force field by adjusting hydrogen atom positions.
RADIATION= Default: RADIATION=CU	CU MO etc...	Radiation setting. CU: Copper K α 1 (Wavelength: 1.54059290 Å) MO: Molibden K α 1 (Wavelength: 0.70931715 Å)
RADIATION_WAVELENGTH=	ff.ff	Definition of a wave length of radiation. Example : If you want to use Copper K α 1 radiation for calculating diffractogram, set up as follows. RADIATION_WAVELENGTH=1.54059290
TWOTHETA= Default: TWOTHETA=(6.0,40.0,0.02)	(f1, f2, f3)	Range of 2 θ and incremental step width settings. f1: Starting point in degree f2: Terminal point in degree f3: Incremental step width in degree
INTENSITY_SCALING= Default: INTENSITY_SCALING=10000.0	ff.ff	Definition of a value of highest intensity in the diffraction peaks.
PVOIGT_ETA= Default: PVOIGT_ETA=0.5	f.ff	Definition of a value of Lorentz-polarization factor in the pseudo-voigt function.
PVOIGT_HK= Default: PVOIGT_HK=0.1	f.ff	Definition of a value of full width at half maximum in the pseudo-voigt function.

Crystal Structure Prediction related keyword

Keyword	Options	Description
CRYSTAL_SEARCH		Crystal structure prediction will be performed.
CSP_MODE= Default: CSP_MODE=MOLECULE	CRYSTAL MOLECULE	When the experimental crystal structure is used as an input for a crystal structure prediction, CSP_MODE should be set to CRYSTAL. Trial crystal structures will be generated by rotating molecule(s) in asymmetric unit. Space group, lattice constants, molecular spatial position in asymmetric unit of the trial crystal structures will be set to them of the experimental crystal structure. When the isolated molecule or molecular complex (not crystal) is used as an input for a crystal structure prediction, CSP_MODE should be set to MOLECULE.
CSP_SEARCH= Default: CSP_SEARCH=ENERGY	ENERGY POWDER_PATTERN	Predicted crystal structures will be ranked according to their crystal energies. The predicted crystal structure with the smallest crystal energy is 1st rank. Predicted crystal structures will be ranked according to their similarities between calculated powder patterns of the predicted crystal structures and previously-inputted powder pattern. The predicted crystal structure with the highest similarity is 1st rank.
CSP_LATTICE=	(a, b, c, α , β , γ)	Lattice constants of trial crystal structures generated in a crystal structure prediction will be set to these values. When this keyword is used, the lattice constants are fixed in the crystal structure prediction. Therefore, the atomic positions in a unit cell will be predicted.
CSP_LATTICE_RESTRAIN		Lattice constants are not optimized in a crystal structure prediction.
CSP_LATTICE_NORESTRAIN		Lattice constants are optimized in a crystal structure prediction.
CSP_SPGP= Default: CSP_SPGP=(P21/C,P212121)	P1 P21 P212121 etc...	Definition of search space within space group symmetry. If you want to run a prediction in search space within P21/c, P212121, and P21 space group symmetries, CSP_SPGP=(P21/C,P212121,P21) should be wrote in an ini file.
CSP_MAX_CRYSTAL=	n	Definition of number of trial crystal structures generated in a process of crystal structure prediction. Default: CSP_MAX_CRYSTAL=200
CSP_LIMIT_MAXCRYSTAL=	n	Definition of limit value for number of trial crystal structures generated in a process of crystal structure prediction. Default: CSP_LIMIT_MAXCRYSTAL=30000
CSP_RSTEP=	ff.ff	Step width in degree for performing molecular rotation. Default: CSP_RSTEP=30.0
CSP_RUN_SEED=	-n	Random seed setting. This value must be set to a negative number. Default: CSP_RUN_SEED=-1000
CSP_PREOPT= Default: CSP_PREOPT=ON	ON OFF	Definition of optimization for inputted structure before performing a crystal structure prediction. ON: Inputted structure will be optimized. OFF: Inputted structure is not optimized.

Keyword	Options	Description
CSP_DEBUG=	INITIAL	Trial crystal structures generated in a crystal structure prediction will be outputted as CIF file format.
	FINAL	Optimized crystal structure will be outputted as CIF file format, when its optimization is completed in a process of crystal structure prediction.
CSP_ROT_MODE= Default: CSP_ROT_MODE=RANDOM		Selection of crystal structure prediction method for performing molecular rotation.
	RANDOM	Molecule(s) in an asymmetric unit will be rotated randomly in a θ_1 range of 0 to 360, a θ_2 range of 0 to 360, and a θ_3 range of 0 to 180. (Step width in the ranges is defined by CSP_RSTEP.)
	GRID	Molecule(s) in asymmetric unit will be rotated in a θ_1 range of 0 to 360, a θ_2 range of 0 to 360, and a θ_3 range of 0 to 180. (Step width in the ranges is defined by CSP_RSTEP.)
CSP_AUS_MODE= Default: CSP_AUS_MODE=RANDOM		Selection of crystal structure prediction method for deciding initial molecular spatial position in a unit cell.
	RANDOM	Molecular spatial positions will be decided randomly.
	FULL	All available molecular spatial positions within a space group symmetry in the program will be considered.
CSP_RESTART		Previous crystal structure prediction, which was stopped before ending of the prediction, will be restarted.
CSP_REOPT=	ON	ON: The crystal structures that constructed from a restart file will be optimized in a restarted prediction.
	OFF	OFF: The crystal structures that constructed from a restart file are not optimized in a restarted prediction.
CSP_ENERGY		Crystal energies of predicted crystal structures are compared on their spherical crystals with same number of molecules.
CSP_ROT_UNIT=		Definition of treatment of molecule(s) in an asymmetric unit. Default: If CSP_MODE=CRYSTAL, CSP_ROT_UNIT=MOLECULE. If CSP_MODE=MOLECULE, CSP_ROT_UNIT=COMPLEX.
	MOLECULE	The molecule(s) in the asymmetric unit will be rotated respectively in the generation of trial crystal structures.
	COMPLEX	The molecule(s) in the asymmetric unit will be treated as one molecular complex. Thus, molecular rotation will be adapted to the molecular complex.
CSP_NOROT_AXIS=	(n1,n2,n3)	Definition of molecular rotation around x, y, and z axes. n1: molecular rotation setting around x axis. (1 or 0) n2: molecular rotation setting around y axis. (1 or 0) n3: molecular rotation setting around z axis. (1 or 0) 1: molecular rotation around the axis is not performed. 0: molecular rotation around the axis will be performed. If you want to fix molecular orientation around x axis, CSP_NOROT_AXIS should be set to (1,0,0).

Keyword	Options	Description
CSP_NOROT_MOL=	n	A molecule with a molecular id n in an asymmetric unit is not rotated in a generation of trial crystal structures. The molecular ids are decided according to serial numbers of atoms in the molecules in an asymmetric unit.
CSP_ROT_MOL=	n	A molecule with a molecular id n in an asymmetric unit will be rotated in a generation of trial crystal structures. The molecular ids are decided according to serial numbers of atoms in the molecules in an asymmetric unit.
CSP_NOROT_ALLMOL		All molecules in an asymmetric unit are not rotated in a generation of trial crystal structures.
CSP_ROT_ALLMOL		All molecules in an asymmetric unit will be rotated in a generation of trial crystal structures.

NMR Analysis Keyword

Keyword	Options	Description
NMR		NMR- $^3J_{\text{HH}}$ coupling constant calculation based on the Karpuls-Imai equation is performed. All combinations of $^3J_{\text{HH}}$ coupling pairs are automatically listed and calculated.

Constraint Driving Keywords

Keyword	Options	Description
CONSTR_BOND= CONSTR_DIST=	(I,J,STA,TER,STP,FK)	Constraint of distance between I-th and J-th atoms (not necessary bonded) is provided. When start length STA, termination length TER, driving step size STP (Angs) are given appropriately, force constants FK of constraint function is automatically set to 10,000 (kcal/mol/ Angs ²), and then stepwise structural modification along the specified reaction coordinate (I-J distance) will be performed with constraint optimization.
CONSTR_ANGL=	(I,J,K,STA,TER,STP,FK)	Constraint of I-J-K angle (not necessary bonded) is provided. FK is set to 10,000 (kcal/mol/rad ²) as default. When STA, TER, STP angles (deg) are given appropriately, structural modification will be performed with constraint optimization.
CONSTR_TORS=	(I,J,K,L,STA,TER,STP,FK)	Constraint of I-J-K-L torsion (dihedral) angle (not necessary bonded) is provided. FK is set to 1,000 (kcal/mol/rad ²) as default. When STA, TER, STP angles (deg) are given appropriately, bond driving will be performed with constraint optimization.
CONSTR_OOPL=	(I,J,K,L,STA,TER,STP,FK)	Constraint of out-of-plane angle of I-J-K plane (not necessary bonded) and L-th atom is provided. FK is set to 1,000 (kcal/mol/rad ²) as default.
CONSTR_PHI5=	(I,J,K,L,M,STA,TER,STP,FK)	5-membered ring phase angle is provided. FK is set to 1,000 (kcal/mol/rad ²) as default.

Stochastic Kick Keyword

Keyword	Options	Description
KICK		Stochastic Kick method will be applied as a pre-perturbation before the specified optimization. The random seed number is set to the constant "123456789" as the default.
KICK=	n	Constant of the random seed number is specified to n.
KICK_RESET		The random seed number will be changed in each call of random generation. The initial seed number is set to the default number.
KICK_RESET=	n	The random seed number will be changed in each call of random generation. The initial seed number is set to n.
KICK_FACTOR=	f	Size of stochastic kick vector is set to 0.01 Å as the default. If the kick factor "f" is specified, the maximum kick size will be set to 0.01*f Å.

Other Keywords

Keyword	Options	Description
TIME= Example : TIME=10.00D	f.ff	The total CPU time allowed for the current job is limited to f.ff seconds (default). Alternative specifications of the time are T=f.ff D, T=f.ff H, T=f.ff M, which define the time in f.ff days, hours, minutes, respectively. If this TIME keyword is not used, by default the time is 3 days (=259,200 seconds).
DEBUG		Specification of "DEBUG" keyword provides debugging information for all subroutines. "DEBUG" keyword is corresponding to "DEBUG=ALL", see below.
DEBUG=	CONCHK HYBRID DEFINE CLASSALL CLASS[o-8] CLASSPPP SYMM EVAL OPT SCFMO ALL	Debugging information can be provided for the following subroutines: CONCHK, HYBRID, DEFINE, CLASSALL, CLASS[o-8], CLASSPPP, SYMM, EVAL, OPT, ALL, NEWTON. Example : DEBUG=(CONCHK,SYMM)
PRINT= NOPRINT=	INPUT MODE LATEST PARAM SYMM NEGEIG SCFMO	Options are used to specify what information should (or should not) be output.