

CONFLEX 6.0 New Features

- Crystal structure calculation method has been added.
- It is now possible to calculate the crystal structure based on an original algorithm developed at Conflex Corporation. CONFLEX 6.0 can optimize the variety of structures derived from a difference of conformations or orientations of molecule. This is useful for studying the energies of crystal polymorphism.
- Improvement of solvent model used in CONFLEX
It is now possible to utilize the GB/SA model for structure optimization, vibrational analysis and conformational search. These calculations must use the MMFF94s force field option in CONFLEX 6.0
- The stabilization energy with solvation can be calculated by the automatic optimization of the molecular structure both in the gas phase and solvent model.
- The functionality of replacement of amino acid residue (PDB file option).
If a Protein Data Bank file is used as input, user can specify the replacement of amino acid residue. This can do a homology modeling-like calculation. Also, this can complement incomplete amino acid residues in a PDB file. If the PDB file is incomplete, CONFLEX 6.0 generates an error message.
- Improvement of conformational search option.
User can now specify the step size of the Stepwise Rotation perturbation in CONFLEX 6.0. This enables a user to do a conformational search of polymers in a limited sense
- Addition of MMFF94s parameters
We have developed and add our own parameters for MMFF94s. This increased the range of molecules which CONFLEX can calculate.
- The Frontier Mode Following Method is added.
FMF method is one of the transition state search method based on a similar technique of the eigenvectors following method.