CONFLEX
HIGH PERFORMANCE
Conformation Analysis

CONFLEX® 7
Conformation Analysis System

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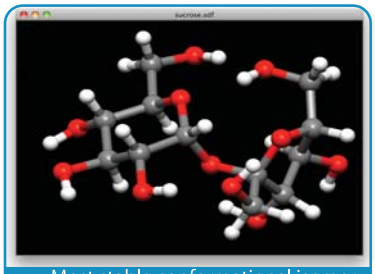
CONFLEX® 7 permits fast, accurate, automated conformation searching and analysis critical to drug discovery and chemical engineering. Unique to CONFLEX 7 is its capability to completely search the conformational space of a flexible molecule to find every optimal structure of chemically significant conformers.

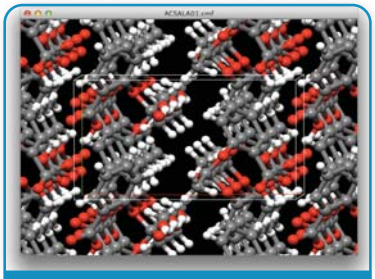
CONFLEX 7 also includes algorithms for predicting vibrational frequencies, thermodynamic properties, CD/UV/Vis spectra, and 3JHH NMR coupling constants.

Utilizing several unique strategies, CONFLEX 7 exhaustively searches conformational space to identify the most stable structures using:

- Stepwise perturbations
- Three perturbation modes to mimic thermal vibration:
  - Stepwise Bond Rotation
  - Edge Flip
  - Corner Flap
- User-selectable force fields
- User-variable search limit



Most stable conformational isomer for sucrose (190.98 kcal/mol)

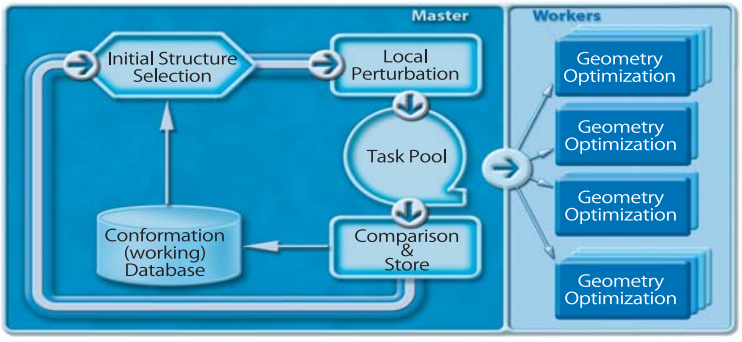


Crystal structure of aspirin

Crystal Search and Optimization

CONFLEX 7 can automatically generate and optimize molecular crystal structures. The energy-minimum structures can be listed in order of not only the energy but also by similarity to prepared powder pattern data.

CONFLEX 7 also calculates powder diffraction data for crystalline structures.



CONFLEX can also be configured for parallel computing environments.

KEY FEATURES & BENEFITS
- Exhaustive conformation searches
- Fast and highly accurate
- Handles small & large molecules
- Single and Parallel CPU options
- CD/UV/VIS Spectra Prediction
- Available as stand-alone engine or with CONFLEX Interface
- Affordable licensing plans

NEW IN THIS RELEASE
- Crystal Search and Optimization
- Powder Diffraction Prediction
- User modifiable force field parameters
- Host-Ligand coordination
- Run from ChemOffice Products
- IR, UV or VCD (Gaussian) Spectral Synthesis based on conformer population

CONFLEX 7 FORCE FIELDS
- MM2
- MMFF94s
- EMM2
- MM3

CONFLEX 7 FILE FORMATS
- mol - MDL molfiles
- sdf - MDL SD File
- pdb - Protein Data Bank File
- log - Gamess Log File
- cmf - Crystallographic Information File
- cif - Crystallographic Information File

SYSTEM REQUIREMENTS
Windows 7 , 8.1 (32bit & 64bit)
Mac OS X 10.8 - 10.10
CentOS 6.1-6.6, 7.0
Ubuntu 12.04.3, 14.04

1.0 GHz Processor & up
40 GB Disk Space
Memory 2 GB minimum

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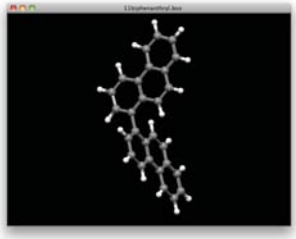
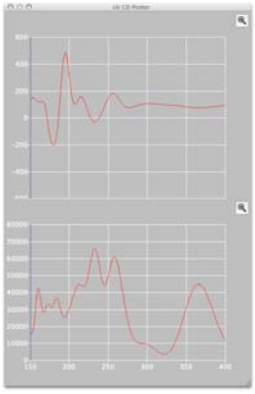
Solvent Effect
CONFLEX utilizes the GB/SA model for geometry optimization, normal mode analysis, and conformational search, as well as for calculating LogP.

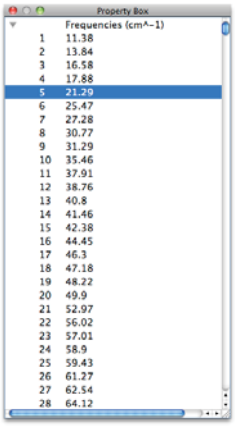
CD/UV/Vis Spectral Analysis
CONFLEX also calculates UV/CD/Vis spectra.

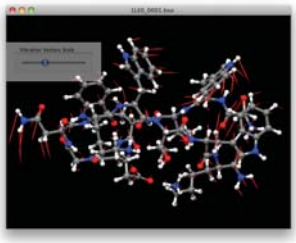




Transition State Structure Search
The frontier mode-following method, which is a modification of the eigenvector-following method, is utilized in CONFLEX for finding transition state structures.

Geometry Optimization
CONFLEX performs a normal mode analysis automatically after geometry optimization, and estimates thermodynamic properties such as Gibbs free energy. CONFLEX also permits partially constraining a structure during geometry optimization.



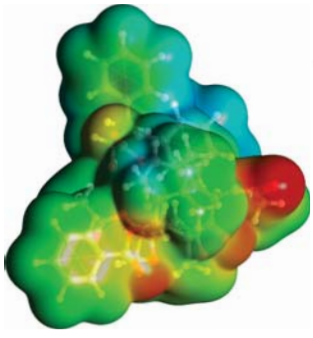


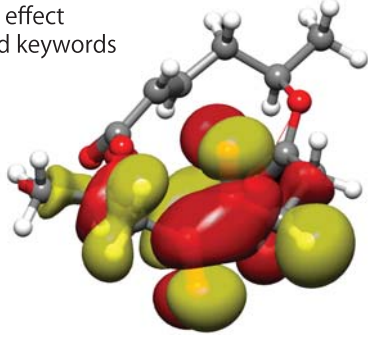
Molecular Object Group Method
The molecular object group that is containing a molecule or a few molecules in a molecular complex system (consisting of some molecules) can be defined, and geometry optimization, normal mode analysis, and conformation search for specified molecular object group are available.

CONFLEX Interface

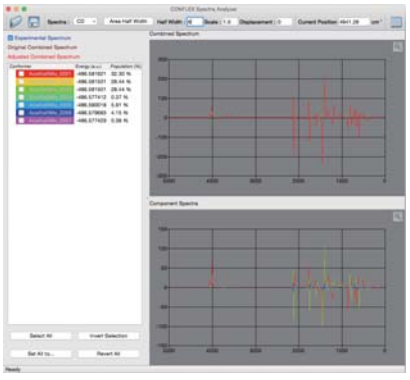
File Formats
- MDL format files: .mol, .sdf
- Sybyl mol2 format
- GAMESS log file
- Firefly log file
- CONFLEX Output file: .bso, .nmr
- Crystallographic Information File format: .cif, .cmf
- Gaussian formatted checkpoint file: .fchk
- Protein Data Bank (PDB) format: .pdb
- Copy & paste from ChemDraw

Calculation Setup & Execution
- Generate calculation input file
- Execute job locally or via network
- Parameter setup for solvent effect
- Easily access frequently used keywords





Calculation Results Display
- View bond distance, bond angle, and torsion angles
- List conformational isomers
- Vector representation for normal mode analysis
- View spectra for IR, NMR, CD/UV/Vis
- Display molecular orbital surface and electron density surface
- Change surface area width in real time
- IR, UV or VCD (Gaussian) Spectral Synthesis based on conformer population



Structure Display
- Display formats: Ball & Stick, CPK
- 3D rotation and zoom
- View bond angles, distance and torsion angles

Third Party Connectivity
Setup and execute jobs for/from:
- Gaussian
- ChemOffice