

Features exported to CDX

Atom properties

The atom properties are exported to CDX file format the following way:

ChemAxon	ChemBioDraw	Comment
Atomic charge	✓	
's<n>' query property except 's*'	✓	Substituents Exactly
's*' query property	✓	Free Sites '*0'
'u' query property	✓	Unsaturation
Reaction Stereo	✓	
Enhanced Stereochemistry	✓	
Radical	✓	
'h<n>' query property except 'h<0>'	✓	Free Sites set to implicit hydrogens on the atom minus n.
'h<0>' query property	✓	Implicit Hydrogens not allowed.
'rb<n>' query property	✓	Ring Bond Count
'H', 'X', 'R', 'r' query properties and Query Valence	✓	Written and read as user defined properties. ChemBioDraw removes them.

Bonds

The following bond features exported to CDX file format from Marvin:

ChemAxon	ChemBioDraw	Comment
Single bond		
Single bond	✓	Plain
Single bond Down	✓	Hashed Wedged
Bold	✓	Bold bond
Single bond Up	✓	Hollow Wedged

Coordinative bond	✓	Dative
Single bond Up or Down	✓	Wavy
Double bonds		
Double bond	✓	Plain
Single or double query bond type	✓	Tautomeric
Aromatic	✓	Aromatic bond
Triple bond	✓	Triple bond
Bond properties		
Query bonds		
Any	✓	Any bond
S/D	✓	Single or double query bond type
S/A	✓	Single or aromatic query bond type
D/A	✓	Double or aromatic query bond type
Topology		
Ring	✓	Bond is in ring
Chain	✓	Bond is in chain
Reaction center		
Center	✓	The bond is a reacting center.
Make/Break	✓	The bond is made or broken in the reaction
Change	✓	The bond (order) has changed in the reaction
Make and Change	✓	The bond is created and changed
Not Center	✓	The bond is not a reacting center
Not modified	✓	The bond is not modified in the reaction

Reaction arrow

The following reaction arrows exported to CDX file format from Marvin:

ChemAxon	ChemBioDraw	Comment
Single reaction arrow type	✓	Solid
Double reaction arrow type	✓	Retrosynthetic
Resonance arrow type	✓	Resonance
Equilibrium arrow type	✓	Equilibrium

Groups

ChemAxon	ChemBioDraw	Comment
Any polymer S-group type	✓	Anypolymer (anyp)
Component S-group type	✓	Component (c)
Copolymer S-group type	✓	Copolymer (co)
Copolymer S-group type with alternating polymer S-group subtype	✓	Copolymer, alternating (alt)
Copolymer S-group type with block polymer S-group subtype	✓	Copolymer, block (blk)
Copolymer S-group type with random polymer S-group subtype	✓	Copolymer, random (ran)
Crosslink S-group type	✓	Crosslink (xl)
Generic S-group type	✓	Generic ()
Graft S-group type	✓	Graft (grf)
Mer S-group type	✓	Mer (mer)
Formulation S-group type.	✓	Mixture, ordered (f)
Mixture S-group type	✓	Mixture, unordered (mix)
Modification S-group type	✓	Modification (mod)
Monomer S-group type	✓	Monomer (mon)
Multiple group S-group type	✓	Multiple Group (#)

SRU S-group type	✓	SRU (n)
Repeat pattern		
Head-to-tail S-group connectivity	✓	Head-to-Tail
Head-to-head S-group connectivity	✓	Head-to-Head
Either unknown S-group connectivity	✓	Either/Unknown
Flip Type	✓	Supported

Symbols

ChemAxon	ChemBioDraw	Comment
LP atoms	✓	Exported as graphical Lone Pairs
Absolute stereo	✓	Exported as 'Abs' label