Features imported from CDX and CDXML files

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Atoms

The atom features from the CDX file format import limitations are the following:

ChemBioDraw	ChemAxon	Comment
Charge	✓	
Isotope	✓	
Isotopic Abundance	✗	
Substituents up to	✓	's<n>' query property up to 6
Substituents Exactly	✓	's<n>' query property up to 6
Free Sites	✓	*0 is converted to 's*', others are converted to 's<n>', calculated: Free Sites-number of bonds.

Unsaturation	✓	'u' query property if set to 'Must be absent'
Reaction Change	✗	
Reaction Stereo	✓	
Translation	✗	
Abnormal Valence	✗	
Enhanced Stereochemistry	✓	
Radical	✓	
Implicit Hydrogens	✓	If not allowed, the atom gets a 'h0' query property
Ring Bond Count	✓	
Hdot / HDash	✓	Imported as explicit hydrogens

Generic labels

The generic labels from the CDX file format are imported to Marvin as:

Label	ChemDraw	ChemAxon
A	Any Atom	Any atom type
M	Metal	Pseudo atom: M

Q	Non-hydrogen heteroatom	Hetero atom type
X	Halogen	Pseudo atom type
R	Unspecified	R-group atom type

Bonds

The following bond features from the CDX file format are imported to Marvin as:

ChemBioDraw	ChemAxon	Comment
Single bond		
Plain	✓	Single bond
Dashed	✓	Single bond Down
Hashed	✓	Hashed
Hashed Wedged	✓	Singe bond Down
Bold	✓	Bold bond
Bold Wedged	✓	Single bond Up
Hollow Wedged	✓	Single bond Up
Dative	✓	Coordinative bond
Wavy	✓	Single bond Up or Down
Double bonds		
Plain	✓	Double bond
Bold	✓	Double bond
Double Either	✓	Double bond

Tautomeric	✔	Single or double query bond type
Aromatic	✔	Aromatic bond
Triple bond	✔	Triple bond
Quadruple bond	✔	Any 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
Ring or Chain	✔	No topology
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 from the CDX file format are imported to Marvin as:

ChemBioDraw	ChemAxon	Comment
Solid	✔	Single reaction arrow type
Bold	✔	Single reaction arrow type
Dashed	✔	Single reaction arrow type
One-Sided	✔	Single reaction arrow type

Hollow	✔	Single reaction arrow type
No Go	✔	Single reaction arrow type
Retrosynthetic	✔	Double reaction arrow type
Resonance	✔	Resonance arrow type
Equilibrium	✔	Equilibrium arrow type
Degree arrows	✔	Not yet supported, will be converted to electron flows

Note that files containing multi-step reactions are imported with graphical arrows, thus these won't be recognized as single reactions in Marvin.

Groups

The following groups from the CDX file format are imported to Marvin as:

ChemBioDraw	ChemAxon	ChemAxon
Bracket Usage		
Unspecified	✔	Generic S-group type
Anypolymer (anyp)	✔	Any polymer S-group type

Component (c)	✔	Component S-group type
Copolymer (co)	✔	Copolymer S-group type
Copolymer, alternating (alt)	✔	Copolymer S-group type with alternating polymer S-group subtype
Copolymer, block (blk)	✔	Copolymer S-group type with block polymer S-group subtype
Copolymer, random (ran)	✔	Copolymer S-group type with random polymer S-group subtype
Crosslink (xl)	✔	Crosslink S-group type
Generic ()	✔	Generic S-group type
Graft (grf)	✔	Graft S-group type
Mer (mer)	✔	Mer S-group type
Mixture, ordered (f)	✔	Formulation S-group type.

Mixture, unordered (mix)	✅	Mixture S-group type
Modification (mod)	✅	Modification S-group type
Monomer (mon)	✅	Monomer S-group type
Multiple Group (#)	✅	Multiple group S-group type
SRU (n)	✅	SRU S-group type
Repeat pattern		
Head-to-Tail	✅	Head-to-tail S-group connectivity
Head-to-Head	✅	Head-to-head S-group connectivity
Either /Unknown	✅	Either unknown S-group connectivity
Flip Type	✅	Supported

Symbols

ChemBioDraw	ChemAxon	ChemAxon

Lone Pairs	✅	Imported as lone pairs, but automatic lone pair calculation writes them over. It can be turned off *e.g.* in MarvinSketch at the Edit > Preferences... > Structure tab.
Abs label	✅	If there is a label in the cdx file, the absolute stereo flag is set to the molecule.

Complex graphics

ChemBioDraw	ChemAxon	ChemAxon
Tables	✅	Tables are imported as graphical objects. The cell size and relative positions are retained, and the cells visualized by rectangles.

TLC plates	✅	TLC plate drawing is imported with graphical elements, keeping original positions.