Features imported from SKC files

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Atom features

The following atom features from the SKC file format are imported to Marvin:

ISIS/Draw	Marvin	Comment
General properties		
Type	✓	
Isotope	✓	
Charge	✓	
Radical	✓	
Valence	✓	
Hydrogen display	✗	
Atom number	✓	*imported as atom map*
Number position	✗	
Value	✓	
Pseudo	✗	
Alias	✗	

Beilstein	✓	*(imported as Pseudo atom)*
Map	✓	
Query properties		
No Implicit Hydrogens	✓	*Imported as* *'Number of implicit hydrogens=0'*
Unsaturated atoms *(Unsaturated bond to atom)*	✓	
Exact change [reaction]	✗	
Ring bond count	✓	*r** imported as *rb**
Reaction stereo	✓	
Enhanced stereo	✓	
Prevent hydrogen substituents	✓	
Allow these atoms	✓	*imported as Atom List*
Prohibit these atoms	✓	*imported as Atom Not List*
Font properties		
Font, size, bold, italic	✓	
Underline, formula	✗	
Atom color	✓	

Bond features

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

ISIS/Draw	Marvin	Comment
Bond type		
Single	✓	
Double	✓	
Triple	✓	
Up	✓	*(Single Up)*
Down	✓	*(Single Down)*
Either	✓	*(Single Up or Down)*
Dbl Either	✓	*(Double Cis or Trans)*
Any	✓	
Aromatic	✓	
Single/Double	✓	*(Single or Double)*
Double /Aromatic	✓	*(Double or Aromatic)*
Single /Aromatic	✓	*(Single or Aromatic)*
Reacting center		
Center	✓	
Make/Break	✓	
Change	✓	
Make/Change	✓	
Not Center	✓	
Topology		

Ring	✓	
Chain	✓	
Other		
Stereo search	✓	
Thickness	✓	
Color	✓	
Crossed bond	✓	

Reaction features

The following reaction features from the SKC file format are imported to Marvin as:

ISIS/Draw	Marvin	Comment
Reaction arrow	✓	*some types of reaction arrows are converted to single reaction arrows*
Reactant	✓	
Product	✓	
Agent	✓	
Multiple step reaction	✗	*converted to graphic arrows*
Reaction and R-group combination	✓	
Reaction and S-group combination	✓	
Resonance	✓	*Resonance arrow type*

Equilibrium	✓	*Equilibrium arrow type*
Degree arrows	✗	*converted to electron flows*

Note that only one reaction arrow per file is imported because Marvin does not support multistep reactions yet.

Group features

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

ISIS/Draw	Marvin	Comment
S-groups		
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)	✔	*Mixture 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)	✔	*Label and bracket type supported, repeat pattern not yet supported*
Superatom S-group	✔	
Repeating unit with repetition ranges(e.g.2,4-6)	✔	
Attached data	✔	
R-groups		
R-group	✔	
Attachment points	✔	
R-Logic	✔	

Graphical objects

All graphical objects except for graphic arc and smooth spline are supported. Line style and Polygon Fill Color are not supported. All text box attributes are imported except for Underlined.

Generic labels

All generic labels are imported to Marvin:

- Any atom (*A*)
- Any atom except carbon (*Q*)
- Any Metal (*M*)
- Any halogen (*X*)
- Any Generic
- Acyclic
- Acyclic hetero
- Acyclic alkenyl
- Acyclic Carbacyclic
- Alkoxy
- Alkyl
- Alkynyl
- Aryl
- Cyclic
- Carbocyclic
- Cycloalkenyl
- Cycloalkyl
- Heteroaryl
- Heterocyclic
- Cyclic no carbon

Attach data

Import of Data to Atom, Data to Bond, Data to Molecule and Data to Brackets is supported.

Chemistry

Import of Autoname, Link node, Create Chiral Flag and residue is supported.

Chirality

Import of CHIRAL and AND attributes is supported.

Known Issues

The import of the following features has not been implemented yet:

- Multicenter bond,
- Position variation bond,
- Hydrogen bond
- Coodination bond
- Variable Repeat Group