



Sketch - Creating and Modifying Models

Molecular models in *iSpartan* are created as standard 2D perspective drawings. Only a few simple tools are needed to create and edit complex drawings.

Tapping on the **Sketch** icon for the first time brings up a palette of icons and buttons ("Sketch palette") and a blank white drawing area ("screen"). Drawings are created by tapping atom or group icons in the palette and then tapping or drawing on the screen. Selecting **C** and drawing CC bonds with your finger or stylus allows you to sketch a complete structural "skeleton" much in the same way you would draw this using pencil and paper. Additional labels, like atom type, stereochemistry, and formal charge, are easily added by tapping the icon that matches the label and then double-tapping the label's location in the drawing.


There is considerable flexibility in the order in which the skeleton and the labels can be drawn. Also, standard 2D perspective cues can be used to create models with well-defined 3D geometries.




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

Sketch Palette. The Sketch palette contains tools for making and manipulating drawings. There are also tools for adding cues to designate stereochemistry and set limits for a substructure search.



The palette (below) contains several components: **defined atoms**, **user-definable atom/functional group**, **common rings**, **common carbonyl groups**, **stereochemical markers** (one type of marker does not actually appear in the palette, but can be added in drawings as desired), **open-site markers**, **charge/radical markers**, and **drawing tools**.




The palette can be repositioned anywhere on the screen by **dragging** it with one finger. It can also be hidden/displayed by **tapping** on any .







1. **Defined atoms.** H, B, C, N, O, F, Si, P, Cl, Br and I only.
2. **User-definable atom/functional group.** This icon is initially designated **Ele/Grp**. **Tap** this icon to bring up a keyboard and **type** a standard chemical symbol. The user-defined symbol can represent an element, e.g., **Na** or **Al**, or a standard group, e.g., **Ph**, **OCH₃**, **OMe**, **NO₂**, or **TMS** (about 60 functional group symbols are presently recognized; a list is found under [Available Groups](#)). The meaning of this icon can be changed by **double-tapping** the icon and entering a new symbol. Case is not important, e.g., **sn**, **sN**, **Sn** and **SN** are all interpreted as **Sn**.
3. **Common rings.** Three icons facilitate the rapid addition of benzene () , cyclohexane () and cyclopentane () rings to drawings.

4. **Common carbonyl groups.** Three icons facilitate the rapid addition of carbonyl () , carboxylic acid/ester () and amide () groups to drawings.





5. **Stereochemical markers.** Wedges and dashes, represented by  and , can be used to designate in-out stereochemistry. Once a stereochemical marker has been added to a drawing, it is possible to designate the orientation of hydrogen atoms and/or substituents bonded to six-member rings as **ax(ial)** or **eq(uatorial)** (*ax* and *eq* labels appear only on the drawing, not in the palette).

6. **Open-site markers.**  designates an “open-site” in a drawing. Searching the database (or its subset) will return all structures with any atoms (including hydrogen) or groups in open sites.

7. **Charge/radical markers.** Conventional bonding rules (neutral C makes 4 bonds, neutral N makes 3 bonds, and so on) are enforced when 2D perspective drawings are converted into 3D models. This is accomplished by adding hydrogen atoms to the drawing so that the bonding rules are obeyed. For example, drawings consisting of only **C** or **N** will be converted into 3D models of CH₄ and NH₃, respectively. (Hydrogen atoms are added to nitrogen, oxygen, phosphorous and sulfur in the 2D drawings.) When another outcome is desired, for example, for an ion or free radical, charge or radical markers must be added to the drawing.

Two icons,  and , are used to label atoms that bear formal charges.  is used to label atoms that are neutral, open-shell radicals. Each of these markers affects the number of electrons and the number of hydrogen atoms added to the 3D model. For example, **O** will produce a 3D model of water, H₂O. However, adding the appropriate marker will result in 3D models of H₃O⁺ () , HO⁻ () , or HO radical () , respectively. (Hydrogen atoms attached to N, O, P and S will also appear in the 2D drawing.) Only one charge/radical marker can be assigned to an atom.

Only one charge/radical marker is displayed on the palette, but tapping the icon will cause each marker to appear in turn.

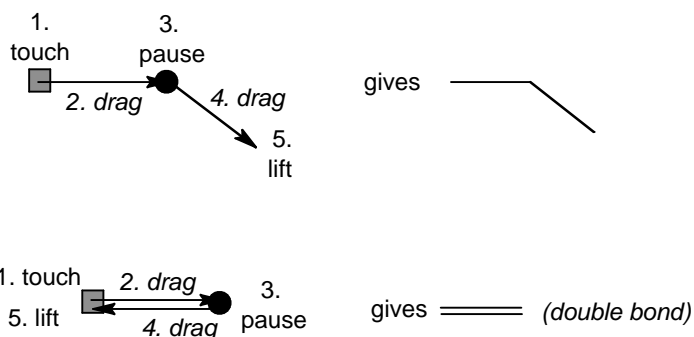
8. **Drawing tools.**  undoes the most recent drawing operation.  removes or modifies parts of a drawing.  deletes an entire drawing (a warning is provided).  tries to improve the readability of a drawing by applying various “clean up” procedures.

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How to use Sketch. **Sketch** is used to create and modify standard 2D perspective drawings. The “skeleton” or network of chemical bonds is drawn by moving a finger (or stylus) across the white portion of the screen in much the same way one draws with paper and pencil. The following terms describe two types of frequently used drawing motions.

Draw. This action combines three actions (**touch-drag-lift**): one **touches** the screen where the drawing should begin, **drags** a finger across the screen to create the desired drawing, and then **lifts** the finger from the screen to signal the end of the drawing. **Draw** can be used to add atoms, common rings, and functional groups.

Draw-pause-draw-... This action combines two or more **draw** actions to create chains and rings of identical atoms. The **lift** action that normally ends each **draw** is replaced by a brief **pause** in which the finger rests on the screen before **dragging** in a new direction (see drawing). **Lifting** the finger after the final **draw** signals the end of the drawing. **Draw-pause-draw** can be used to draw chains and multiple bonds as shown below. It can also be used to draw rings (not shown).



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

How to start drawing. A drawing can be started in several ways:

1. **Tap** the icon for an atom (or common ring, or carbonyl group) that is to appear in the drawing. **Double tap** the screen. Just that atom (or ring, or group) will appear.

2. **Draw** a CC bond that is to appear in the drawing. You can also use this technique with other atoms. For example, to start with an NN bond, **tap N** and **draw**.
3. The drawing technique in #2 can also be used to create chains and rings of identical atoms. To draw an all-carbon chain or ring, **draw** the first bond, **pause** briefly **without lifting**, and then **draw** the next bond in a new direction. **Draw-pause-draw-pause-...** can be repeated as many times as you like. The chain will terminate when you **lift** your finger.

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How to add an atom, ring, or carbonyl group. A drawing can be added to in several ways:

1. To add an atom, **tap** that atom's icon. **Touch** the atom in the drawing that will connect to the new atom and **draw** a bond starting from this location.
2. To add a chain of identical atoms, begin as in #1, then use **draw-pause-draw-pause-...** to create a chain of bonds. This technique can also be used to add rings of any size to a drawing. Simply **draw** the last bond in the chain to an atom that already appears in the drawing.
3. To add a common ring acid/ester, amide or carbonyl group, **tap** that ring's (group's) icon, **touch** the atom in the drawing that will connect to the new ring (group) and **draw** a bond starting from this location. The carboxylic acid/ester  and amide  icons contain an arrow that shows which atom in these groups will be connected to the existing drawing. To change the location of this connection point (arrow), **tap** the group's icon until the arrow reaches the desired location.

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How to draw multiple bonds. To add a multiple bond, first **draw** a single bond at the location where the multiple bond is needed, then **redraw** this line once to make a double bond, and **redraw** it again to make a triple bond (in other words, **touch** one end of bond, **drag** to other end, and **lift**).

The **draw** and **redraw** operations can also be combined and performed as **draw-pause-draw....** To draw a double bond, **draw** a single bond, **pause** without lifting, then

re-draw the bond in the reverse direction. To draw a triple bond, add another **pause-draw**....

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How to fuse 5 and 6-member rings. **Tap** an icon for the first ring and **double tap** the screen. Next, **tap** the icon for the second ring and **double tap** the **bond** that the rings will share. This will create a drawing with a fused bicyclic ring system. Note that the (*cis* or *trans*) stereochemistry of the ring juncture may be ill-defined.


This technique can also be used to add 5 and 6-member rings to an existing bond in any drawing. **Tap** the icon for the ring to be added and **double tap** the **bond** that will become part of the ring.

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How to replace one atom with another. If a drawing contains atom A where atom B is needed, **tap** the icon for B, then **double tap** A in the drawing.

This simplifies the drawing of heterocycles. First, draw an all-carbon ring and then replace specific carbons with heteroatoms.

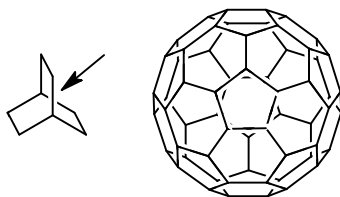
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How to define and add a non-standard element or group. **Tap** the icon underneath H and B (this icon will initially be labeled **Ele/Grp**, but the label will be replaced each time you specify a new element or group). To define an element, **type** the one or two-letter standard chemical symbol for the element and **tap return**. To define a group, **type** the atoms in the group (e.g., **OCH3** or **NO2**) or a standard abbreviation for the group (e.g., **OMe**, **Ph**, or **TMS**) and **tap return**. Case is not important, e.g., **sn**, **sN**, **Sn** and **SN** are all interpreted as **Sn**. Characters will appear in the icon in the palette as soon as you type them. Sequences in red are not recognized (either the group is unknown to *iSpartan* or you have not finished typing), whereas recognizable sequences will appear in green. **Tap** on  and then on **Available Groups** to see the list of available groups.

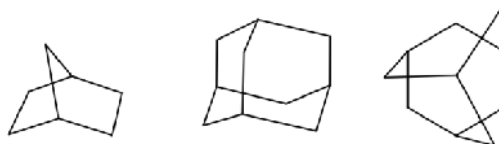
The element/group can be added to a drawing, replaced, or removed using the same drawing techniques used for standard atoms. The element/group can also be redefined. **Double tap** the icon and **type** the symbol for the new group.

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How to draw one bond “in front of” or “behind” another. Conventional perspective drawings use “broken” bonds to show that one bond passes behind another. For example, the broken bond in bicyclo[2.2.0]octane (arrow, left structure) lies behind the vertical CC bond. The same “broken bond” technique is used many times in a fullerene drawing (right structure).


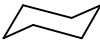

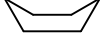
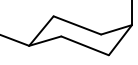
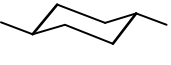


“Broken bonds” are **not used** in *iSpartan*. When one bond crosses in front of or behind another, simply **draw** the new bond across the other. The following drawings are converted into correct 3D models of bicyclo[2.1.0]heptane (left structure) and adamantane (center and right structures), respectively.





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How to draw 3D perspective with line drawings. *iSpartan* attempts to account for intended perspective and orientation when converting 2D drawings into 3D models. The examples in the following table show how this capability can be exploited. Note, that the intended structure might not be realized in every case, and the user should carefully examine the 3D model. More reliable control of stereochemistry and 3D geometry can be achieved using **stereochemical markers**.


2D sketch	3D model	2D drawing	3D model
	<i>cis</i> -2-butene		<i>chair</i> cyclohexane
	<i>trans</i> -2-butene		<i>twist boat</i> cyclohexane
	<i>cis</i> -1,4-dimethylcyclohexane		<i>trans</i> -1,4-dimethylcyclohexane

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How to add stereochemical markers (dashes, wedge). 3D information can be added to a drawing by replacing single bonds with stereochemical markers: dashes or wedge. The single bond must be drawn before a marker can be added.



To replace a single bond with a marker, **tap** either  or , then **re-draw** the single bond. To reverse the orientation of the marker, **re-draw** the bond or marker in the opposite direction.

One type of marker can be replaced directly by the other. **Tap** the desired marker and then **re-draw** the existing marker.

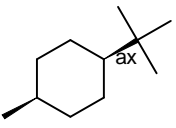
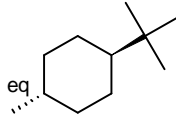
Markers can also be converted back into single bonds. **Tap** , then **double tap** the marker once.

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How to add a axial or equatorial marker (6-member rings only). The orientation of a hydrogen/substituent on a 6-member ring can be specified by marking **one** ring substituent as either **ax(ial)** or **eq(uatorial)** (if a molecule contains multiple rings, the conformation of each ring can be specified by marking **one** substituent per ring). *Axial* or *equatorial* markers can only be added to stereochemical markers (dashes, wedge) so the bond connecting the substituent to the ring must be drawn with a stereochemical marker first.

To add an *axial* or *equatorial* marker to a stereochemical marker, **tap** either  or , then **double tap** the stereochemical marker. **ax** will appear on top of the stereochemical marker. To replace **ax** with **eq**, **double tap** the stereochemical marker again. To remove **eq**, **double tap** the marker again.

Although it is possible to produce a drawing in which several bonds are marked as *axial* or *equatorial*, **iSpartan** uses **only one** marker when converting a 2D ring drawing into a 3D model. For best results during 2D-to-3D conversion, all substituent bonds to the ring should be drawn with stereochemical markers.

2D sketch	3D model
	<i>cis</i> -1- <i>tert</i> -butyl-4-methylcyclohexane (<i>axial tert</i> -butyl)
	<i>trans</i> -1- <i>tert</i> -butyl-4-methylcyclohexane (<i>equatorial methyl</i>)





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How to draw Haworth projections (edge-on) rings. Haworth projections are commonly used to represent carbohydrate rings from an “edge-on” perspective. These projections can be created in **iSpartan** using the  stereochemical marker. First, **draw** the ring using **single bonds**. Next, **tap**  and **re-draw** the **two single bonds** that appear as wedges in a Haworth projection (see drawing). The ring bond separating these “wedge bonds” will automatically be converted into a heavier bond consistent with an “edge-on” perspective. This perspective will also be used to convert the 2D drawing into a 3D model.



This method for adding “edge-on” perspective with wedges can be applied to a variety of structures, including acyclic chains. Dashes cannot be used for “edge-on” perspective.

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How to assign charges, unpaired electrons, and the number of “added” hydrogens. Formal charges and unpaired electrons can be assigned to individual atoms using charge/unpaired electron markers. To assign a **positive** formal charge to an atom, **tap**  and **double tap** the atom in the drawing. To assign a **negative** formal charge or **unpaired electron**, **tap** the charge/unpaired electron marker until the desired icon appears (tapping the marker rotates it through three possibilities: , , and ) and **double tap** the atom in the drawing.


The charge/unpaired electron marker on an atom can be changed in two ways. 1) To **replace** one marker with another, **tap** the desired charge/unpaired electron icon and **double tap** the marked atom. 2) To **remove** a marker, **tap**  and **double tap** the marker.

Charge/unpaired electron markers play an important role during the conversion of 2D drawings into 3D models in that they determine the number of hydrogens that get added to the model (it is usually unnecessary to draw hydrogens in drawings unless they are needed to mark stereochemistry).

Hydrogens are not shown in 2D perspective drawings unless they have been drawn explicitly (exceptions: hydrogens attached to neutral N, O, P, and S are shown automatically). When a drawing is converted into a 3D model, hydrogens are added to the model according to conventional bonding rules. A neutral carbon atom is assumed to form four bonds, nitrogen three bonds, oxygen two bonds, and so on. Analogous logic is used for atoms that carry a formal charge or unpaired electron marker.

Charge and unpaired electron markers also affect how a 3D model is treated during modeling calculations. The total charge is set equal to the sum of the formal charges in the 2D drawing. A model with one unpaired electron is treated as a free radical (drawings that contain more than one unpaired electron may give unanticipated results).


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How to specify “open site” marker(s) for a database substructure search. To mark an “open site” for a substructure search on the database, **tap** , locate the atom in the drawing that will carry the open site, and **draw** a bond starting from this location. As many open site markers as desired may be added to the drawing.

To remove an “open site” marker, **tap**  , then **double tap** the ? marker in the drawing.

Database searches are performed as **exact** searches when no open sites are marked in the 2D drawing. A “match” is returned only if every atom in the search drawing matches up with the same type of atom in the model in the database. **Substructure** searches are performed whenever one or more open sites are marked in the search drawing. A “match” can be returned regardless of what atom(s) (including hydrogen) in the database match up with the open site.



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How to undo the last action. **Tap**  to return to the drawing as it existed before the last action. Earlier versions of the drawing cannot be accessed.



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How to adjust a drawing’s appearance (size, screen position, orientation). All manipulations of 2D drawings involve two-finger gestures. To increase the size of the drawing, **spread** two fingers over the drawing. To reduce the size, **pinch** two fingers over the drawing. To move the drawing around the screen, **drag** two fingers around the screen (left-right or up-down). To rotate the drawing in the plane of the screen, **twist** two fingers over the drawing.


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How to “clean up” a drawing. **Tap**  to improve (“clean up”) the appearance of a 2D drawing and make it easier to read in the Gallery. Note, that not every “clean up” will produce a desirable result. **Tap**  to undo an unsatisfactory “clean up”.


An additional “clean up” operation involves a “2D conformation search”. This allows rotation about single bonds (in 2D) to extend multi-atom chains in an attempt to move

atoms to less crowded positions in the drawing. To access, first, **long press** on  and then **tap**  in the resulting menu. Once again, not every “clean up” will produce a desirable drawing.


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How to remove an atom or bond. **Tap**  and then **double tap** the atom or bond. Note that if you tap an atom, all bonds to that atom will also be removed. Removing a bond, either by tapping an atom or by tapping the bond itself, will also remove terminal atoms, that is, atoms not connected to any other atoms in the drawing will be removed along with the bond.



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How to reduce the bond order of a bond. To reduce the bond order of a (multiple) bond, **tap**  then **double tap** the multiple bond. This reduces the bond order by one. Repeated double taps on a triple bond will reduce the bond order: triple → double → single → no bond.

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How to remove a stereochemical marker (dash or wedge). **Tap** , then **double tap** the marker. This replaces the marker with a single bond.

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How to change or remove an axial or equatorial label from a stereochemical marker. **Tap** either  or , and then **double tap** the stereochemical marker where

an *axial* or *equatorial* label appears. This cycles the label (in order) among **ax** (*axial*), **eq** (*equatorial*) and nothing. The stereochemical marker itself will not be affected.


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How to remove formal charge & unpaired electron markers. Tap  and **double tap** the marker.


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How to remove “open site” markers. Tap  and **double tap** the ? marker in the drawing. **Substructure** searches of the database are performed only if one or more “open site” markers appear in a 2D drawing. **Exact** searches are the default when a drawing does not contain open sites.

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How to clear the screen for a new drawing (start over). Tap . A warning message will ask you to confirm this operation.

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How to convert a drawing into a 3D model. Tap  at the bottom of the screen. The molecular mechanics calculation used to optimize atom positions (the 3D geometry) may take a few seconds if the model is relatively large and/or flexible. If the expected delay is longer than a few seconds, a “progress bar” will appear at the bottom of the screen and a **Stop Minimizer** button will appear at the top of the screen. You can **tap** the latter to stop the minimizer and provide a 3D structure. In this case, note that the


structure provided is not completely optimized, and there is no way to resume the molecular mechanics calculation.

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How to save a drawing in the Gallery for later use. Tap  at the bottom of the screen, (optionally) provide a name and **tap Save**. This will add the drawing to the **Gallery** and simultaneously shift the app into **Gallery** mode. If you do not provide a name, the molecular formula will be used, e.g., C₂H₆O. You can rename the drawing in the **Gallery** using the **Edit** feature.

If you **tap Don't Save** instead of **Save**, you can inspect all of the drawings and models in the **Gallery**, but the current drawing will not be saved in the **Gallery**.


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How to open a drawing from the Gallery. Tap , locate and **double tap** on the drawing of interest.


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How to take a photo of a drawing. Tap  at the top right of the screen and select **Save Sketch in Photo Gallery** from the menu. Photos can be accessed using the **Photos** app.

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How to e-mail a drawing. Tap  at the top right of the screen and select **e-mail Sketch** from the menu.

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How to perform a substructure search on the database. (Landscape mode on the iPad is preferred over portrait mode for this operation.) Following specification of "open site" markers (see [How to specify "open-site" marker\(s\) for a database substructure search](#)), **tap**  at the bottom of the screen. Searching will begin immediately. To terminate the search before it has completed, **tap** on **Cancel** at the top right of "**Search Hits**". To remove the search, **pull down** on the list of search hits. When the search has completed (or terminated), **tap** on an entry to see its structure. In landscape mode, both the list of search hits and structure of the selected molecule are shown together on screen. To see a different entry, simply tap on it in the list. In portrait mode (and on the iPhone), the list and structure are not simultaneously displayed. Tap on an entry to see its structure and on **Search Hits** at the top left of the screen to go back to the list of search hits. Having selected a structure, **tap** on **3D** at the bottom of the screen to view properties, spectra and graphics for this model.

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