Theory in bond calculation

Bond criteria

The Calculate Bonds tool creates bonds between two atoms if the following criteria are met:

- Neither of the two atoms is excluded from forming bonds, i.e. they are not elements in the element exclusion list.
- The sum of the covalent radii of the two atoms fulfills the bond-length criterion below.

$TolFac_{lower} \times ideal\ distance < distance < TolFac_{upper} \times ideal\ distance$

where

distance= distance between the two atoms forming the bond.

$TolFac_{lower}$ = lower tolerance factor. The lower tolerance factor is set using the Bond-length tolerance options on the Bond Calculation dialog.

$TolFac_{upper}$ = upper tolerance factor. The upper tolerance factor is set using the Bond-length tolerance options on the Bond Calculation dialog.

ideal distance = R_{cov}(Atom1) + R_{cov}(Atom2) and R_{cov} denotes the covalent radius of the atom.

Calculating Bonds

The Calculate Bonds tool uses the following procedure:

1. Tests all selected bonds and all bonds attached to a selected atom for compliance with the bond criteria. Deletes non-compliant bonds.
2. Creates atom pairs using all selected atoms and their symmetry images on one side and the whole structure on the other.
3. Forms bonds between all pairs that fulfill the bond criteria.
4. Calculates bond types for all selected and newly created bonds.
5. Converts the display style of resonant bonds to either Kekulé or resonant representation.

Note. If no objects are selected in a structure the bond calculation includes all atoms and bonds.

Monitoring Bonds

The bond monitor is used to automatically recalculate bonds if the document is modified. The bond monitor triggers a bond calculation if one of the events in the following list occurs:

- The selection is changed

- The value of a bond criteria is changed or a new bonding scheme is loaded
- The element type of an atom changes
- An atom changes position
- An atom or bond is deleted or added

Further information

Calculating bonds
Bond Calculation dialog
Element Exclusion List dialog (atoms that are excluded from covalent bonds)
Default bonding schemes

Default bonding schemes

The default bonding schemes provide the most commonly used criteria for the formation of chemical bonds. The first three sets; No bonding to s- and f-shell, No bonding to d- shell, and Include all elements, differ in the set of elements *not* forming chemical bonds.

The last two sets; Tetrahedral and Anions, are intended for special visualization of atomic arrangements within a sublattice of tetrahedral bonded atoms or within an anion sublattice, respectively. This may be particularly useful for zeolite structures.

Name	Bond-length tolerance		Elements excluded from bonding
	min	max	
No bonding to s- and f-shell (default)	0.6	1.15	1st row elements (Li-Fr) 2nd row elements (Be-Ra) Lanthanide elements
No bonding to d-shell	0.6	1.15	As above + transition metal elements
Include all elements	0.6	1.15	None
Tetrahedral	0.6	1.5	Oxygen, sulfur
Anions	0.6	2	Aluminum, silicon, phosphorus