The notion of covalency dates back to the very early days of quantum chemistry:

"We shall denote by the term "covalence" the number of pairs of electrons which a given atom shares with its neighbors" (Langmuir, 1919)

It is an equally crucial but also fuzzy concept in chemistry.

The transition between covalent bond and non-covalent interactions is continuous.

This carries over to the transition between inter- and intramolecular.

Chemical visualization software draw bonds based solely on pre-defined interatomic distances.

Examples of continuous change from covalent to non-covalent bonds

\[ \text{S}_2\text{2 reaction:} \]

\[ \begin{align*}
\text{Nu} & \rightarrow \text{Nu} \\
\end{align*} \]

Hydrogen shift in oxalic acid with increasing pressure:

Formation of intermolecular pnictogen, chalcogen, and halogen bonds due to covalent contributions


Complexes between DABCO and R-Br electrophiles: changing from 1.946 Å in F₅Pyr-Br⁺ to 3.154 Å in CH₂Br(NH₂)

C-C distance in bridged annulenes:

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Intermolecular covalent interactions

Bonds in GaussView Cont.

When no connectivity info present, GV infers bonding:

- Determined from GV table of atomic pair distances
- Used for the Clean function
- Customizable via GV Preferences (Expert feature)

Expected bonds appear to be "missing" in unusual structures

Use distance+chemical intuition to determine whether bond interaction exists