

Chemical Bond, from the Quantum Theory of Atoms in Molecules

Dr. Cina Foroutan-Nejad

Currently, bonding analysis of molecules based on the Quantum Theory of Atoms in Molecules (QTAIM) is popular; however, “misinterpretations” of the QTAIM analysis are also very frequent. In this contribution the chemical relevance of the bond path as one of the key topological entities emerging from the QTAIM’s topological analysis of the one-electron density is reconsidered. The role of nuclear vibrations on the topological analysis is investigated demonstrating that the bond paths are not indicators of chemical bonds. Also, it is argued that the detection of the bond paths is not necessary for the “interaction” to be present between two atoms in a molecule. The conceptual disentanglement of chemical bonds/interactions from the bonds paths, which are alternatively termed “line paths” in this contribution, dismisses many superficial inconsistencies. Such inconsistencies emerge from the presence/absence of the line paths in places of a molecule in which chemical intuition or alternative bonding analysis does not support the presence/absence of a chemical bond. Moreover, computational QTAIM studies have been performed on some “problematic” molecules, which were considered previously by other authors, and the role of nuclear vibrations on presence/absence of the line paths is studied demonstrating that a bonding pattern consistent with other theoretical schemes appears after a careful QTAIM analysis and a new “interpretation” of data is performed.