Discovering Chemical Structure with Linus Pauling

Jin H. Kim
Parkland College

Recommended Citation
Kim, Jin H., "Discovering Chemical Structure with Linus Pauling" (2019). Natural Sciences Poster Sessions. 159.
https://spark.parkland.edu/nsps/159

Open access to this Poster is brought to you by Parkland College's institutional repository, SPARK: Scholarship at Parkland. For more information, please contact spark@parkland.edu.
Discovering Chemical Structure

Linus Pauling

Linus Pauling Biography

- Born February 28, 1897, Portland, Oregon.
- B.S. in chemistry, 1919; Ph.D., 1922.
- Assistant Professor of Chemistry, 1922-1925.
- Professor of Chemistry, 1925-1935.

Early history of structural chemistry

- Edward Frankland (1852) introduced concept of valence.
- Alexander Graham (1861) used term structural chemistry.
- Alfred Werner (1914) explained octahedral configuration of transition metal complexes.
- J.H. van 't Hoff (1874) formulated the octet rule for the valence of the carbon atom.
- Gilbert N. Lewis (1916) discovered the covalent bond and the theory of valence bond structure.
- Lewis introduced the concept of valence electrons.

Introduction to Quantum Mechanics

- Heitler and London (1927) applied quantum mechanics to chemical problems.
- Pauling applied quantum mechanics to the structure of molecules.

Nature of the chemical bond

- Orbital hybridization:
  - Carbon atom has four equivalent bonds even though it has one 2p orbital and three 2p orbitals.
  - For example, the structure of water molecule.

Electronegativity

- Electronegativity map:
  - The electronegativity of elements is related to the ionic character of the formed bond.
  - Elements with high electronegativity tend to attract electrons more strongly.

Resonance

- Further detailed information about the chemical bond resulted from a consideration of the energy of single bonds in relation to the relative electronegativity of the bonded atoms.
  - The ionic character of the bond increases with the difference in electronegativity.

Example of covalent bonding

- The hybridization of atomic orbitals is needed to describe the bonding in molecules.
  - For example, the benzene molecule.

Structure of metallic compounds

- Unlike other compounds, larger number of bonding electrons are used in the transition metal compounds.
  - For instance, iron can be illustrated as having six valence electrons, which occupy hybrid spd orbitals.

- Pauling reported the idea of the structure of transition metal compounds by using the concept of valence bond theory.

- Metallic orbitals have been found of value through the discussion of the properties of metallic and intermetallic compounds.

References


Structure of organic compound

- The isomeristic distances and bond angles in the polypeptide chains of proteins are precisely known to within about 0.1 and 2° respectively.

- Extensive numerical calculation was necessary to make hydrogen bonding structures of polypeptide due to the requirements of planar amidic group and reducing amidic repulsions.

- Pauling has proposed two stereochemically equivalent hydrogen bonding helical structures for a polypeptide chain with 3.7 and 3.5 residues per turn, respectively.

- This has shown the value of the use of structural arguments that go beyond those of the classical structure theory of organic chemistry.