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If Physics Doesn't Work, try Math: Understanding Chemistry using Graph Theory. I.D. Brown, Brockhouse Inst. for Materials Research, McMaster Univ., Hamilton, Ontario, Canada L8S 4M1.

The molecular bond diagrams that are so popular among chemists are mathematical graphs comprising vertices (atoms) and edges (bonds). They allow both organic and inorganic structures to be analyzed using graph theory with a minimal number of chemical assumptions. These assumptions include the coordination number and formal charge (valence) of the atoms and the strength (valence) of the bonds, the latter correlating with the bond length. The model assumes that the bond valence is equal to the valence each atom contributes to the bond, that consistent with this the valence is uniformly distributed between the bonds except for bonds between atoms of similar electronegativity which have a valence of 1.0. Unlike the analysis of bonds in terms of electron densities and orbitals, graph theory does not require an a priori knowledge of the structure or geometry, and furthermore it is simple, quantitative and predictive.