
PATRICK W. FOWLER, University of Sheffield, UK

The Chemical Significance of Graph Energy

Energy is a well-defined physical quantity with discrepant definitions in the mathematical chemistry of π systems. In an extensive mathematical literature, graph energy, $E_G(G)$, is the sum of absolute values of adjacency eigenvalues of graph G . This is a tractable but imperfect mimic of the physical Hückel energy, $E_\pi(G, N)$, a quantity that depends on both G , the molecular graph of the conjugated carbon framework, and the π electron count, N . Discrepancies between $E_G(G)$ and $E_\pi(G, N)$ can be arbitrarily large, but we reconcile the two definitions with a natural connection to the chemical concept of bond number.