doi:10.1351/goldbook.MT07068

maximum hardness, principle of

A chemical system at a given temperature will evolve to a configuration of maximum absolute hardness, η, provided that the potential due to the nuclei, plus any external potential and the electronic chemical potential, remain constant. In terms of molecular orbital theory, the highest value of η reflects the highest possible energy gap between the lowest unoccupied and highest occupied molecular orbitals; this value correlates with the stability (***See:*** structural stability; electronic stability) of a system.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1950

