

**maximum hardness, principle of**

A chemical system at a given temperature will evolve to a configuration of maximum absolute hardness,  $\eta$ , 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  $\eta$  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, thermodynamic stability and kinetic stability) of a system.

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