A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M = H, Li, Na) systems

Contreras, R.

Safont, V. S.

Pérez, P.

Andrés, J.

Moliner, V.

Tapia, O.

Semiempirical Amsterdam Density Functional (ADF) and ab-initio (B3LYP) density functional theory (DFT) calculations are used to analyze the isomerization reaction MCN ? MNC, for M = H, Li and Na systems. A molecular similarity parameter defined in terms of the activation hardness is used to discuss the Hammond rule, relating the ground and transition state structures found in the potential energy surfaces (PES). The maximum hardness principle (MHP) and a local hard-soft acid and base (HSAB) principles are examined for each process. Solvent effects on the isomerization barrier and DFT reactivity indices are also examined at an ab-initio level.

Keywords: Isomerization reactions; density functional analysis of isomerization reactions; molecular similarity in isomerization reactions; solvent effects in isometization reactions.