

Nitro/*Ac*i Tautomerization

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Abstract

It is well established that nitroalkanes and nitroaromatics can undergo a tautomerization in which a hydrogen is transferred from a methyl, hydroxyl or amino group to an oxygen of a nitro group. The resulting tautomer is known as an *aci* form of the original molecule, or alternatively as a nitronic acid. The *aci* tautomers are generally significantly less stable than the parent nitro compounds. *Ac*i tautomerization is believed to be an initial step in the detonation decomposition of some energetic compounds, and thus related to their sensitivities to unintended detonation initiation. In the present work, we look at the transition states and energetics of several nitro \rightarrow *aci* tautomerizations.