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## Research Details:

Research Title : <u>Transition states of some pyridines</u>

Transition states of some pyridines

Description : Geometry and energy of the transition states using Synchronous

Guided Quasi-Newton (STQN) method of the transformation of pyridine-2-(1H)-one to pyridine-2-ol, pyridine-2-(1H)-thione to

pyridine-2-thiol and 1,2-dihydro-2-iminopyridine to 2-

aminopyridine were investigated using ab-initio MO method at the level of 6-31G\*\* + MP2. The mechanism of transformation between reactants and products can be followed using 1,3-segmatropic rearrangement and conjugated dual hydrogen bonding (CDHB)

complex formation.

Research Type : Article Research Year : 2002

Publisher : ASIAN JOURNAL OF CHEMISTRY Volume: 14 Issue: 2 Pages: 889-

897

Supervisor : Al-Thabaiti SA, Al-Nowaiser FM

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## Researchers:

Researcher Name (Arabic) Researcher Name (English) Researcher Type Degree Email

أ.د. شعيل بن احمد الثبيتي

Al-Thabaiti SA

Researcher

أستاذ

فوزية محمد النويصر

Al-Nowaiser FM

Researcher