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Estimation of transition state and Synthesis of Barbituric Acid with their derivatives of 1,3,4-Thiadiazole

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ABSTRACT

Quantum calculation method have been used to estimate the real transition state for the synthesis of Barbituric Acid and their derivatives of 1,3,4-Thiadiazole using semiemperical calculation methods. Optimized structures, electronic transition spectrum and vibration spectrum have been calculated for the preparative compounds compared with their experimental spectrums. Theoretical examination of transition state has been done to know the real transition state of reaction through zero point energy, total binding energy and first imaginary frequency. Three suggested transition states have been proposed for the reaction of 2-amino-5-mercapto-1, 3, 4-thiadiazol with 4-dimethylamino benzaldehyde. First transition state is the real state due their energy values comparatively with other states. Barbituric Acid and some of new derivatives of 1, 3, 4-Thiadiazol have been prepared as new medical agents. Good agreements has been found between the experimental and theoretical spectrums for the synthetic products, likes N-{5-(2, 2-Dimethylisopropylidenyl) thio-1,3,4-thiadiazolyl}-N-Benzoyl-amino-(4-(N-Dimethylamino)benzyl–aminobarbituric acid as final product.

Keywords: Quantum calculation methods, transition states, Barbituric Acid, Thiadiazole Semi-empirical and PM_3.
