Turkish Journal of Chemistry

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Chemistry

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A New Method for the Preparation of Pyridazine Systems: Experimental Data and Semiempirical PM3 Calculations

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Abstract: The reactions of 4-benzoyl-5-phenyl-2,3-furandione (1a) and 4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-2,3-furandione (1b) with acyl hydrazines (2) (namely hydrazides) are reported. From these reactions, novel pyridazinone systems (3a-g) are obtained as well as the cyclization product of 3g at high temperature (4). The electronic properties and conformational parameters for these molecules, such as bond lengths, bond angles, torsion angles and atom charges, are calculated with a semiempirical PM3 method. In order to determine the mechanism of the reaction between the model furandion (R1) and formic hydrazide (R2), the electronic properties, conformational parameters and imaginary frequencies of the reactants, transition states and intermediates are calculated at the same level of theory as well.

Key Words: Hydrazide, furandione, pyridazine, semiempirical, PM3

Turk. J. Chem., **30**, (2006), 691-701.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.30,iss.6.