THEORETICAL STUDY OF THE CONFORMATIONAL STRUCTURE AND THERMODYNAMIC PROPERTIES OF 5-(4-OXO-1,3-THIAZOLIDINE-2-YLIDENE)-RHODANINE AND ETHYL-5-(4-OXO-1,3-THIAZOLIDINE-2-YLIDENE)-RHODANINE-3′-ACETIC ACID AS ACCEPTOR GROUPS OF INDOLINE DYES

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The quantum chemical DFT method with the B3LYP hybrid functional in 6-31++G(*d*,*p*) and 6-311+G(*d*,*p*) basis sets is used to calculate the equilibrium geometric parameters of different conformations of 5-(4-oxo-1,3-thiazolidine-2-ylidene)-rhodanine and its substituted form ethyl-5-(4-oxo-1,3-thiazolidine-2-ylidene)-rhodanine-3′-acetic acid applied in the synthesis of indoline and some other sensitizing dyes for solar cells. The thermodynamic parameters of four conformers and their synthesis reactions are calculated. The effect of substituents on the thermodynamic stability of the studied isomers is shown.

Keywords: indoline dyes, rhodanine, birhodanines, density functional theory, enthalpy of formation.