

ORIGINAL PAPER

Effect of reactants' concentration on the ratio and yield of *E,Z* isomers of isatin-3-(4-phenyl)semicarbazone and *N*-methy lisatin-3-(4-phenyl)semicarbazone^aKlaudia Jakusová*, ^bMartin Gáplovský, ^aJana Donovalová, ^aMarek Cigáň,
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Dedicated to Professor Štefan Toma on the occasion of his 75th birthday

In this work, the effect of inter- and intramolecular interactions of reactants and products, reactants concentration as well as the solvent effect on the ratio of *E* and *Z* isomers of isatin-phenylsemicarbazones in the reaction mixture is examined. Theoretical calculations proved that *Z* isomers are more stable than *E* isomers. Experimental results confirmed the noncovalent intermolecular donor-acceptor interactions of the reactants in the reaction mixture at concentrations above 0.1 mol L⁻¹. The *E/Z* isomer ratio of isatin-3-(4-phenyl)semicarbazone (*I*) and *N*-methy lisatin-3-(4-phenyl)semicarbazone (*II*) depends on the initial concentrations of 3-amino-1-phenylurea (phenylsemicarbazide; *V*) and 1*H*-indole-2,3-dione (isatin; *III*), or 3-methy lindol-2,3(1*H*)-dion (3-methy lisatin; *IV*), respectively. Both isomers exhibit high thermal stability. Thermal *E-Z* isomerization takes place at temperatures above 70 °C in *N,N*-dimethy lformamide.

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Introduction

Considerable attention has recently been paid to the preparation of compounds which can be subjected to photoisomerization for their practical application in electronics, e.g. switches, storage media, and sensors. Inter- and intramolecular interactions, especially hydrogen bonds as relatively weak interactions, play an important role in biology; they affect, amongst other things, the course of chemical reactions and also the stability and structure of compounds. The information on their existence and their characteristics in the studied system often helps to understand the molecule's physical and chemical properties (Cubero et al., 1999;

Senthilkumar et al., 2005). Formation of these hydrogen bonds often leads to hydrogen transfer from a hydroxy or amino group to the acceptor, especially in biological and photochemical processes (Levy, 1980; Li & Fang, 2003; Otsubo et al., 2002). The transfer of hydrogen (or proton) from the base or excited state of a molecule occurs in both the solution and the solid phase (Li & Fang, 2003; Alarcón et al., 1995; Falkovskaia et al., 2002; Mehata et al., 2002; Chai et al., 2005).

Inter- or intramolecular hydrogen bonds represent a very important group of interactions which affect the physico-chemical properties of compounds. The change of physico-chemical properties of chemical

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