Identification of Two Hetero-Substituent-Aromatic Isomers of - 4- and 7-Hydroxy Coumarin with the Belousov-Zhabotinsky Oscillator

Muhammad Yasir Nawabi¹, Waqar Uddin¹, Gang Hu^{1&2*}, Saif Ullah¹,
Zhaohui Fang³ and Saira Sardar⁴

¹ Department of Chemistry, Anhui University, Hefei, 230601, People's Republic of China

² Anhui Province Key Laboratory of chemistry for Inorganic/Organic Hybrid Functionalized Materials

³ The First Affiliated hospital of Anhui University of Chinese Medicine, Hefei, 230031, P. R. China.

⁴ Institute of Chemical Sciences, University of Peshawar, Pakistan

*E-mail: hugang@ustc.edu

doi: 10.20964/2019.09.08

Received: 8 May 2019 / Accepted: 17 June 2019 / Published: 31 July 2019

In this article, we presented an innovative work of distinguishing the two different positional hetero-substituents-aromatic isomers i.e. 4-hydroxycoumarin (4-HC) and 7-hydroxycoumarin (7-HC) on their perturbation effect by a novel analytical Belousov-Zhabotinskii (BZ) oscillator. In such BZ oscillator, the tetra-aza-macrocyclic copper complex ($[\text{CuL}](\text{ClO}_4)_2$) was used in which the ligand L is 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11 diene. Experimental data confirmed that, by discrete injection of these two isomers (4-HC and 7-HC) into the active BZ system with equal concentrations reflected in their inhibition time (t_{in}), but the t_{in} produced by 4-HC was higher than the t_{in} initiated by 7-HC. The interesting feature is that, with increasing concentrations (9.0×10^{-5} to 3.6×10^{-4}) of 4-HC constantly increase the t_{in} and decreased the oscillation number (N) after the regeneration of oscillation. Whereas, the upsurge concentrations of 7-HC didn't change the t_{in} but reduced the N after regeneration of oscillation. Thus, the two isomers were identified. Based on the mechanistic approach of FKN (Field-Koros-Noyes) model, the reaction perturbation mechanism was discussed. A fleeting description is that both 4-HC and 7-HC isomers were oxidized by $\text{BrO}_2^\bullet$ intermediate radical (which produce during the course of reaction) into salicylic acid and quinone respectively and the system was temporary freeze (t_{in}) as well. The products (salicylic acid and quinone) were identified by infra-red and Ultra-Visible spectroscopies.

Keywords: Belousov-Zhabotinsky; Chemical Oscillation; Isomers Identification; Hydroxycoumarin; Intermediate Species; Perturbation effect

[FULL TEXT](#)

© 2019 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).