Crystal Structure and Electrochemical Properties of 1-(4bromophenyl)-ferrocene-prop-2-en-1-one and 1-(3-(4bromophenyl)-5-(ferrocene)-4.5-dihydropyrazol-1-yl) ethenone

Naved Azum^{1,2*}, Muhammad Nadeem Arshad^{1,2}, Abdulhadi Salih Birinji¹, Khalid A. Al-Amry¹, Abdullah M. Asiri^{1,2}, Layla Ahmad Taib¹, Yasser Mohammed Al Angari¹, Sher Bahadar Khan^{1,2}, Antonio Facchetti^{3*}

¹Chemistry Department, Faculty of Science, King Abdulaziz University, P. O. Box 80203, Jeddah 21589, Saudi Arabia.

²Center of Excellence for Advanced Materials Research (CEAMR), King Abdulaziz University, P. O. Box 80203, Jeddah 21589, Saudi Arabia. ³Flexterra Corp., 8025 Lamon Avenue, Skokie IL, 60077, USA

*E-mail: <u>navedazum@gmail.com</u>, <u>afacchetti@flexterracorp.com</u>

doi: 10.20964/2019.09.47

Received: 18 April 2019/ Accepted: 6 July 2019 / Published: 31 July 2019

Compounds having redox-active ferrocenyl groups have attracted considerable interest in several branches of Chemistry and Materials Science. Here we investigate a chalcone (compound I) having a ferrocenyl group which is further derivatized to pyrazoline to achieve a hybrid molecule having a ferrocenyl couple to a heterocyclic ring (compound II). These compounds were characterized using spectroscopic techniques including the (¹H-NMR and ¹³C-NMR), UV–Visible and infrared (FT-IR) studies to confirm the structures and investigate the electronic properties of I and II. Furthermore, we confirmed the three-dimensional structures and any relevant interactions among the molecules in their unit cells using single crystal X-ray diffraction analysis. The molecules of both compounds stabilized by the C-H...halogen interactions, where Br acts as a halogen atom. Finally, the redox properties of I and II were accessed by cyclic voltammetry experiments. It is observed that the chalcone derivative has larger oxidation potential than the pyrazoline derivative.

Keywords: Synthesis, Ferrocene, Pyrazoline

FULL TEXT

© 2019 The Authors. Published by ESG (<u>www.electrochemsci.org</u>). 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/).