عنوان مقاله:

Theoretical predict the electrochemical oxidation behaviour of some para diamine species using results of the electrochemical oxidation of 4- aminodiphenylamine

محل انتشار:

بیست و یکمین کنفرانس شیمی فیزیک انجمن شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Electrochemical studies of amines were performed by numerous workers at variousconditions such as aqueous and non-aqueous solvent or at various pHs [1]. It was reported thatelectrochemical oxidation of aromatic amines is quite complex, and leads to a variety of productsdepending on their structure and electrolysis conditions [2]. The reported results indicated thathydrolization can occur in electrochemical oxidation of some amines, and rate of the hydrolysisis dependent to pH and the structure of molecule [3]. It was reported that amines with morepositive oxidation potential (EpA1) have larger ΔGtot values and there is a linear relation betweenthese parameters [4]. In this work firstly using the oxidation potential of 4-aminodiphenylamine(1) in pH=7 and calculated ΔGtot of it, and calculated ΔGtot studied diamine derivatives (2-9),oxidation potentials of the species (2-9) were estimated. The electrochemical oxidation of paradiamine species indicates that these species convert to their p-quinone dimines via two electronprocess. Reported results show that electrogenerated p-quinone dimines participate in thehydrolysis reaction and are converted to their p-benzoquinones and rate of hydrolysisdependence to N=C bond orders. Secondly using structure of 4-aminodiphenylamine (1) in pH=1and its NBO analysis rate of hydrolysis reaction for all studied species (1-9) were compared witheach other. All calculations were performed using Density Functional Theory (DFT) B3LYPlevel of .theory and 6-311G (p,d) basis set

کلمات کلیدی:

Para diamine species, Electrochemical oxidation, Δgtot

لینک ثابت مقاله در پایگاه سیویلیکا: