

New approach to electrochemical reactivity of aniline tetramer through a combined view of DFT and CV descriptors.

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Rok wydania

2018

Czasopismo

Synthetic Metals

Numer woluminu

242

Strony

8-16

DOI

10.1016/j.synthmet.2018.04.006

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The phenyl/ NH_2 -terminated aniline tetramer was synthesized chemically. The quasi-reversible cyclic voltammetry (CV) curves of its oxidation in strong aqueous trihalogenoacetic acids was confronted with relevant density functional theory (DFT) calculations by assuming step-wise proton-electron (PE) and/or electron proton (EP) elementary reactions. The CV experimental and DFT theoretical standard potentials as well as the kinetic measures (CV peak separations and dependence on the scan rate) and the DFT theoretical reorganization energies were compared. The P_0EPEP and P_0EE mechanisms of the elementary reactions were postulated for the overall two-electron quasi-reversible oxidation of aniline tetramer in trifluoroacetic acid and tribromoacetic/trichloroacetic acids, respectively, where P_0 is acid-neutral tetramer complex formation involving interaction through H-bonds. The molecular structures of the tetramer-acid complexes involved in the oxidation/reduction process were shown and characterized by their density functional theory (DFT) descriptors. A combination of DFT and CV results allowed to simulate CV characteristics that agreed with that observed experimentally.

Słowa kluczowe

Aniline tetramer (TANI), Aqueous trichloroacetic acids ($\text{F}_3\text{C}-\text{COOH}$, $\text{Cl}_3\text{C}-\text{COOH}$, $\text{Br}_3\text{C}-\text{COOH}$), Density functional theory (DFT), Cyclic voltammetry (CV)

Adres publiczny

<https://doi.org/10.1016/j.synthmet.2018.04.006>

Strona internetowa wydawcy

<http://www.elsevier.com>