DFT estimates of water environment impact on the reversible $2e^{-}$ + $2H^{+}$ oxidation of aniline tetramer.

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The PCM (IEFPCM) and CPCM implicit models of water environment have been embodied to the DFT calculations of the reversible $2e^{-}$ + $2H^{+}$ process of aniline tetramer. The molecular structure of six reactants as well as reaction energy characteristics of their six reactions have been determined and compared to the vacuum model. The clear difference in reaction energy between two types of processes, electron transfers and proton transfers, is the advantage of the solvent model approach in comparison to the most simple gas phase calculations. The results corresponding to the electron transfer reactions, namely the redox potentials, are much closer to empirical expectations than DFT determinations done for the vacuum environment of the isolated tetramer.

Słowa kluczowe

density functional theory, Polarizable Continuum Model, Polarizable Conductor Calculation Model, polyaniline, Ionization energy, electron affinity, Reaction energy, Reorganization energy, electrode potentials, redox

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