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A benzopyran based optical sensor for the selective trace determination of Pd (II): Analytical investigation and computational calculations

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Abstract

Determination of palladium is essential owing to the element's toxic ecological effects on biological systems. Due to the element's noxious and amiable characteristics, there has been a great deal of interest in identifying and detecting its presence in a variety of natural as well as commercial samples. Hence, a thorough spectrophotometric investigation is conducted regarding the trace Pd (II) determination in organic phase *via* its reaction with 3-hydroxy-2-phenyl-4*H*-chromen-4-one (HPC), a chromogenic reagent derived from benzopyrans and acting as an optical sensor for the metal to be determined. The optimal reaction conditions for formulation of the intricate structure of the developed complex are depicted, in order to ensure the element's determination. The foundation of this study is based upon sensing Pd (II) by its colour complexation with the sensor, HPC, that resulted into a stable binary yellow complex with a λ_{max} at 417-432 nm. Stoichiometric ratio of the studied Pd (II)-HPC complex as deduced from Job's continuous variations and mole ratio approach has been 1:2 [M:L]. Analytical findings support a square planar geometry of the investigated coordination complex. High reproducibility of the outcomes is further supported by statistical evidences, including attenuation coefficient ($\varepsilon = 1.9159\times10^4$ L mol^{-1} cm^{-1}), standard deviation (SD = ± 0.00184), Sandell's sensitivity (S = 0.0055 µg cm^{-2}), detection limit (LOD = 0.1122 µg mL^{-1}) and regression coefficient (r = 0.9975). A variety of commercial samples have been analysed with remarkable sensitivity, selectivity, accuracy, and precision, under set conditions of the procedure. The theoretical studies have been conducted to enhance our comprehension of the complex's molecular geometry and structural attributes. Density Functional Theory (DFT), with method PBE/def2-TZVP, for quantum chemical computations, successfully assisted in identifying and interpreting chemical behaviour of the acquired Pd (II)-HPC complex elucidating the chemical interactions, its stability and reactivity trends. DFT, has a strong correlation with the analytical research, proving that the studied complex behaves as a strong biological agent. The studied complex was indeed subjected to antimicrobial and antioxidant studies, the results of which reflected that the Pd (II)-HPC complex has a strong potential to act as a strong antimicrobial and a radical scavenging agent.

Keywords: Palladium, Chromen-4-one, Analytical studies, Computational behaviour, Antioxidant, Antimicrobial