Selective copper determination using a sensor based on a vinylferrocene moiety: A theoretical study

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Abstract

The selectivity of (E)-2-[(3-(2-ferrocenyl)vinyl)-5,5-dimethylcyclohex-2-enylidene]malononitrile (FcL) toward different cations was studied theoretically at the DFT level. Ten interaction sites were evaluated, and its energetic and electronic properties analyzed. Ligand to cation charge transfer was obtained in most of the studied complexes, iron acting as the main electron donor. An exception was observed, in which the organic moiety acted as electron donor and both, Fe and cation as acceptors, allowing a bimetallic interaction. The high selectivity of (FcL) ligand towards copper was stablished based on the number of formed complexes, the highest binding energy, and the strong charge transfer towards copper cation. © 2021 Elsevier B.V.

Author keywords

Binding energy; Charge-transfer; Copper sensor; DFT; Vinyl-Ferrocenyl