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Multitask Quantum Study of the Curcumin-Based Complex Physicochemical and Biological Properties

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Abstract: Density functional theory (DFT), time-dependent density functional theory (TDDFT), quantum theory of atoms in molecules (QTAIM), and extended transition state natural orbitals for chemical valence (ETS-NOCV) have all been used to investigate the physicochemical and biological properties of curcumin and three complexes, i.e., Cur-M (M = Ni, Cu, and Mg). Based on DFT calculations, the enolic form (Cur-Enol) is more stable than the anti-diketone form (Cur-Anti diketone) favored for complexation. This enolic form stability was explained by the presence of three intramolecular hydrogen bonds according to the QTAIM analysis. Furthermore, the ETS-NOCV technique revealed that the enolic form had more significant antioxidant activity compared with the anti-diketone form. The calculations from the COnductor-like Screening MOdel for Realistic Solvents (COSMO-RS) showed that the dimethyl sulfoxide (DMSO) solvent could dissolve all the curcumin tautomers Cur-Enol, Cur-Anti-diketone and Cur-Cu, Cur-Mg, and Cur-Ni complexes in contrast to benzene, acetone, octanol, ethanol, methanol, and water. Furthermore, except for Cur-Mg, which had a relatively low solubility (14 g/L), all complexes were insoluble in water. Cur-Anti-diketone was considerably more soluble than Cur-Enol in the examined solvents.

Keywords: curcumin; metal complex; ETS-NOCV; QTAIM; TDDFT; COSMO-RS

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1. Introduction

Curcumin, a major active component of Turmeric, has long been used as a spice, and it possess a wide range of biological activities, including antibacterial and antifungal [1], antioxidant, anticancer [2,3], antimicrobial [4], and inflammatory properties [5]. Curcumin has piqued the interest of many academics since then, and numerous papers have been published on the subject [6–8]. It was first discovered by Vogel and Pelletier as a powder "yellow coloring matter" from rhizomes of *C. longa* (Zingiberaceae family) [9], and characterized and first synthesized by Milobedeska, Lampe et al. [10,11].

The chemical structure was investigated by Heger et al. [12] as [(1*E*, 6*E*)-1,7-bis(4-hydroxy-3-methoxy-phenyl)-1,6-heptadiene-3,5-dione]. Curcumin has a melting point of