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Computational structure characterization, nonlinear optical properties and antitumor activities of Nickel(II) complexes containing alkoxy-derived dicyandiamide ligands

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$[Ni(dcda\text{-}O\text{-}Me)_2]^{2+}$ **(1)**, $[Ni(dcda\text{-}O\text{-}Et)_2]^{2+}$ **(2)**, $[Ni(dcda\text{-}O\text{-}nPr)_2]^{2+}$ **(3)**, and $[Ni(dcda\text{-}O\text{-}nBu)_2]^{2+}$ **(4)** complexes (dcda-O-R is dicyandiamide ligands with alkoxy-derived) have been optimized in the gas phase at B3LYP/LANL2DZ/6-31+G(d,p) level. Computational structure characterization has been performed from the structural parameters, IR spectra, ^{1}H-NMR, ^{13}C-NMR chemical shift values. It has been found that the central metal atom geometry in the complexes is a distorted square plane. Some electronic structure descriptors of the complexes are calculated in the gas phase and nonlinear optical properties are predicted. Complex **1** is found as the most suitable compound to produce optical material. The complexes are optimized at the same level in the aqueous phase to determine antitumor activity. Some electronic structure descriptors are calculated and molecular docking calculations are made against the 3WZE protein. According to the calculated electronic structure descriptors and molecular docking results, it is found that the complex **3** has the highest antitumor activity against the selected target protein.

Keywords: Dicyandiamide, Ni(II) complexes, Computational structure characterization, NLO properties, Antitumor activity

Dicyandiamide (dcda) is a ligand having two tautomeric structures as N≡C–N=C$(NH_2)_2$ and N≡C-NHC(=NH)NH_2. As seen from tautomeric structures, the dcda ligand contains a nitrile group (N≡C-). Nitrile is an active group and forms dicyandiamide derivatives by giving nucleophilic addition reactions with water, alcohols, and amines in the presence of transition metal ions. While guanylurea is formed by the nucleophilic addition of water to dicyandiamide, 1-amidino-O-alkylurea is formed by the nucleophilic addition of alcohols, and biguanides are formed from the nucleophilic addition of amines[1-5]. There is no significant reaction between dicyandiamide and alcohols when there is no metal ion. However, the addition of alcohol to dicyandiamine in the presence of the Cu(II) ion results in high yields, while the same reaction takes a long time in the presence of Ni(II), requires a base, and the yield is low[6,7].

Dicyandiamide and its derivatives form complexes with transition metals. Transition metal complexes have widespread use due to their biological, catalytic, and optical properties. Because of their catalytic properties, they are used as catalysts in many industrial processes such as alkene polymerization[8], olefin metathesis[9], and Wacker process[10]. Due to their biological activities, they are used as antimicrobial, antibacterial, antibiotic, antitumor drugs in the health field[11-16]. Due to their optical properties, they are used in the production of valuable optical materials such as optical modulation, optical switching, optical logic, and optical memory[17,18]. The biological, catalytic, and optical properties of transition metal complexes depend on many factors such as the type of metal, the oxidation state of the metal, the type of ligand, the number of donor atoms of the ligand and the coordination number of the complex. The change in each of these factors gives the complex a different feature and complex activity changes.

The syntheses and molecular structure determination of $[Ni(dcda\text{-}O\text{-}R)_2]^{2+}$ type four-coordinated complexes were reported by Kose et al. Also, it has been experimentally found that complexes have higher antimicrobial activity than ligands against some microorganisms[19]. However, there is no study on nonlinear optical (NLO) properties and antitumor activity of the complexes.

In this study, we aimed to determine the molecular structures of the complexes {$[Ni(dcda\text{-}O\text{-}Me)_2]^{2+}$ **(1)**, $[Ni(dcda\text{-}O\text{-}Et)_2]^{2+}$ **(2)**, $[Ni(dcda\text{-}O\text{-}^{n}Pr)_2]^{2+}$ **(3),** and $[Ni(dcda\text{-}O\text{-}^{n}Bu)_2]^{2+}$ **(4)**} by quantum chemical

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