عنوان مقاله:

Theoretical Investigation of ۴-Methyl-۴H-۱,۲,۴-triazole-۳-thiol and Its Mononuclear and Dinuclear Palladium(II) Complexes; Molecular Structure, NBO Analysis, FT-IR and UV-Vis Spectroscopy

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خلاصه مقاله:

In this research, the characterization of complexes [Pd(aemptrz)Cl۲] (۱), [Pd۲(μ-mptrz)۲(mptrz)۲(en)].CH۳OH (۲) [Pd۲(μ-mptrz)۴] (۳) and [Pd۲(μ-mptrz)۲(mptrz)۲(en)] (۴) (where aemptrz is ۱-(۱-(λ۲-azanyl)ethyl)-۴-methyl-۵-(λ۱-sulfanyl)-۴H-۱λ۴,۲,۴-triazole, en is ethylene diamine and Hmptrz is ۴-methyl-۴H-۱,۲,۴-triazole-۳-thiol) were carried out by Density Functional Theory (DFT) calculations. Structural, electronics and molecular properties (such as bond distances, bond angles, energies of highest occupied molecular orbital (EHOMO), the lowest unoccupied molecular orbital (ELUMO), the energy gap (ΔE), chemical hardness η, the dipole moment μ and Natural bond orbital (NBO) analysis of compounds) have been investigated using B۳LYP/TZVP level of theory. Moreover, electronic structures of all complexes via NBO calculation show that Pd-N and Pd-S bonds are made of delocalization of occupancies from lone pair (LP) orbital of N, S atoms to the palladium atom. The FT-IR spectroscopy analysis and electronic spectra were calculated using B۳LYP/TZVP basis set and compared with the experimental values. Furthermore calculation of vibrational spectra are also allocated based on the potential energy distribution (PED) using the VEDA ۴ program. The .electronic spectra were calculated using DFT and time dependent density functional theory (TD-DFT) methods

کلمات کلیدی:

Methyl-۴H-۱, ۲, ۴-triazole-۳-thiol, Palladium(II) complexes, Energy gap, Chemical hardness η, Dipole moment μ,-۴ Density functional theory (DFT), Potential energy distribution (PED), TD-DFT