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First-Principle Studies of Istradefylline with Emphasis on the Stability, Reactivity, Interactions and Wavefunction-Dependent Properties
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Dermal fibrosis and Parkinson's disease are two chronic syndromes affecting a large population leading to systematic morbidity. The mechanisms of these diseases are well debated, and many medicines are in the market for managing them. Recently, istradefylline was approved by the FDA as a medicine for the management of aforesaid disorders. But the detailed structure and reactivity profile of this compound was not reported. We use molecular modeling using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods using B3LYP/CAM-B3LYP/aug-cc-pVDZ level to study the structure, reactivity and other physicochemical properties of this compound. Conformational analysis over two dihedral angles was discussed. The compound was found to be an ideal candidate for being used as an NLO material. Molar refractivity was found to be 13.19 times greater than urea and 2.61 times greater than p-nitro acetanilide. TD-DFT indicated that the compound shows excellent light-harvesting efficiency of 94.21 in the near UV region of 337.23 nm. We also report several wavefunction-based properties such as molecular electrostatic potential, localized orbital locator, average local ionization energy, local information entropy and electron localized function. Using MESP, LIE, LOL, etc., information entropy studies showed that the molecule is stable with low uncertainty electrons in spatial distribution. These studies are useful for future experimental studies involving istradefylline and will assist in the design and prediction of the activity of new derivatives from this compound.
Keywords: DFT istradefylline LIE local information entropy MESP
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Research Articles

First-Principle Studies of Istradefylline with Emphasis on the Stability, Reactivity, Interactions and Wavefunction-Dependent Properties

Nabil Al-Zaqri, T. Pooventhiran, Ali Alsalme, D. Jagadeeswara Rao, Siriki Srinivasa Rao, A. Sankar & ...show all

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Abstract

Dermal fibrosis and Parkinson's disease are two chronic syndromes affecting a large population leading to systematic morbidity. The mechanisms of these diseases are well debated, and many medicines are in the market for managing them. Recently, istradefylline was approved by the FDA as a medicine for the management of aforesaid disorders. But the detailed structure and reactivity profile of this compound was not reported. We use molecular modeling using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods using B3LYP/CAM-B3LYP/aug-cc-pVDZ level to study the structure, reactivity and other physicochemical properties of this compound. Conformational analysis over two dihedral angles was discussed. The compound was found to be an ideal candidate for being used as an NLO material. Molar refractivity was found to be 13.19 times greater than urea and 2.61 times greater than *p*-nitro acetanilide. TD-DFT indicated that the compound shows excellent light-harvesting efficiency of 94.21 in the near UV region of 337.23 nm. We also report several wavefunction-based properties such as molecular electrostatic potential, localized orbital locator, average local ionization energy, local information entropy and electron localized function. Using MESP, LIE, LOL, etc., information entropy studies showed that the molecule is stable with low uncertainty electrons in spatial distribution. These studies are useful for future experimental studies involving istradefylline and will assist in the design and prediction of the activity of new derivatives from this compound.

Keywords: DFT istradefylline LIE local information entropy MESP

Disclosure statement

There are no conflicts of interest.

Additional information

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УДК 517

Coupled Fixed Point Theorems Via Mixed Monotone Property in A_b-metric Spaces & Applications to Integral Equations

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Abstract. In this paper, we establish some results on the existence and uniqueness of coupled common fixed point theorems in partially ordered A_b-metric spaces. Examples have been provided to justify the relevance of the results obtained through the analysis of extant theorem. Further, we also find application to integral equations via fixed point theorems in A_b-metric spaces.

Keywords: Coupled fixed point, Mixed weakly monotone property, A_b-metric space, Integral equation.

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1. Introduction and preliminaries

The study of fixed point theory comes from wider area of non-linear function analysis. However, its study began almost a century ago in the field of algebraic topology. Fixed point theorems find applications in proving the existence and uniqueness of the solutions of certain differential and integral equations that arise in physical, engineering and other optimization problems. In the study of fixed point theory, some of the generalizations of metric space are 2-metric space, D-metric space, D^*-metric space, G-metric space, S-metric space, Rectangular metric or metric-like space, Partial metric space, Cone metric space. In 1989, I. A. Bakhtin [2] introduced the concept

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