

عنوان مقاله:

Effects of Substituent and Temperature on the Electronic Properties and Thermodynamics Parameters of ۱-(Benzothiazolylamino) Methyl-۲-Naphthol: A Computational Study

محل انتشار:

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نویسندگان:

Zohreh Khanjari - *Department of Chemistry, Karaj Branch, Islamic Azad University, Karaj, Iran*

Bitia Mohtat - *Department of Chemistry, Karaj Branch, Islamic Azad University, Karaj, Iran*

Reza Ghiasi - *Department of Chemistry, Faculty of science, East Tehran Branch, Islamic Azad University, Tehran, IRAN*

Hoorieh Djahaniani - *Department of Chemistry, East Tehran Branch, Islamic Azad University, Tehran, Iran*

.Farahnaz Kargar Behbahani - *Department of Chemistry, Karaj branch, Islamic Azad University, Karaj, Iran*

خلاصه مقاله:

The effects of substituent and temperature on the ۱-(benzothiazolylamino) methyl - ۲-naphthol molecules were studied at CAM-B3LYP/۶-۳۱۱G (d,p) level of theory. Selected substitutions were NH₂, OH, Me, F, Cl, CHO, COOH, CN and NO₂. Substituent effect on the frontier orbitals energies, HOMO-LUMO gap, chemical potential, and electrophilicity were explored. Dependencies of energy changes, reactivity properties and thermodynamics parameters (G, H and S) on the Hammett's constants (p) were provided. Thermodynamics parameters values of the formation reaction were studied reaction at ۱۰۰-۱۰۰۰ K range. Computational investigation of the substituents and temperature influences on the formation reaction of the ۱-(benzothiazolylamino) methyl-۲-naphthol showed the negative E values in the studied reactions. Calculated dipole moment values reveal the presence of the EWGs induced a larger dipole moment compared with the EDGs. Higher negative values were found in the presence of EWGs compared to EDGs. Frontier orbitals were stabilized in the presence of EWGs. However, frontier orbitals were destabilized in the presence of EDGs. Thermodynamic analysis revealed that these reactions were non-spontaneous and exothermic. The G and negative H values were increased with increasing the temperature. Optimization and vibrational analysis were done with Gaussian ۰۹ software package. The standard ۶-۳۱۱G(d,p) basis set was considered for the elements, respectively. CAM-B3LYP functional was used for the optimization of the geometries of the compound. This functional is Handy and coworkers' long range corrected version of B3LYP using the Coulomb-attenuating method. The identities of the optimized structures as an energy minimum were confirmed by vibrational analysis.

کلمات کلیدی:

۱-(Benzothiazolylamino)methyl-۲-naphthol, Substituent effect, Temperature effect, Thermodynamics parameters)

لینک ثابت مقاله در پایگاه سیویلیکا:

