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Stereo-Chemical and Computational Analysis of Luminol Molecule and its Isomers Using Quantum Physical Energy JAE EUN KIM, DAYEON CHEONG, SEWON CINDY PARK, Choice Research Group — Luminol, efficiently used in the field of forensic, medicine, and plant sciences, detects bloodstains at crime scenes and develops biosensors. This research provides theoretical and computational analysis of the luminol molecule and its derivatives. The computational analysis and calculations of optimized energies(kcal/mol) of Luminol's derivatives, which have large role in molecules stability, were carried out based on the electronic density functional analysis. The stabilities based on optimized energies of the conformations of luminol tautomers were presented and the comparisons of the numerical data with the original luminol are given. Through the analysis of stability order, we can confirm the use of electronic density analysis as functional. Also the study confirms the existence of three important factors that influence the relative stability of luminol's tautomers. The first factor is the aromaticity and electronic delocalization, which depends on the number of molecular orbitals of p character. The second is the molecule's hydrogen bonding and the third, and the most important factor, is charge distribution.

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