

عنوان مقاله:

Investigation of the Effect of Substitutions on the Electronic and Optical Properties of the Sumanene Molecule

محل انتشار:

مقالات مروری و پژوهشی شیمی، دوره 6، شماره 4 (سال: 1402)

تعداد صفحات اصل مقاله: 13

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خلاصه مقاله:

Sumanene ($C_{24}H_{12}$) is the smallest bowl-shaped molecule containing a central benzene ring, which is alternately surrounded by another 3 benzene rings and cyclopentadiene rings. In this study, the effect of various electron donor and receptor substitutions on its structure, electrical and optical properties were investigated. The results showed that the electron-bonding and electron-donor-acceptor groups to sumanene greatly affected the electrical properties. In contrast, the most significant effect occurred when NO and CH_2Li substitutions were at the two positions simultaneously. These substitutions also greatly influenced optical properties and significantly increased its polarization and polarization values. The most significant effect occurred when BH_2 and NCH_2Li were replaced in position 1. Finally, the absorption spectrum of the substituted molecules was examined when the BH_2-NCH_2Li groups were in position 1.

کلمات کلیدی:

Sumanene, Orbital Energy, Absorption spectra, Optical properties

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