عنوان مقاله:

Theoretical investigation on the aromaticity of mono-substituted benzene derivatives by using cyclic reference

محل انتشار:

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تعداد صفحات اصل مقاله: 6

نویسنده:

خلاصه مقاله:

The degree of aromaticity of mono-substituted derivatives of benzene has beeninvestigated using a new index based on electric field gradient index, by using two mechanicalquantum methods with Gaussian ۰۳. Two different basis sets have applied to study and theresults compared. This strategy has demonstrated that, due to violation of symmetry in have pisystems,how the degree of aromaticity can have been changed. A comparison of the values ofour aromaticity index with other indices reveals a good correlation for these compounds

کلمات کلیدی:

Mono-substituted benzene, Electrostatic Field Gradient, EFG, Aromaticity