

Electron affinity of the monobromomethyl radical and vibrational spectrum of its anion: a combined coupled-cluster and density functional study.

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Streszczenie

Adiabatic electron affinity (EA) of the CH_2Br radical and vibrational frequencies and inversion barrier of the corresponding anion CH_2Br^- have been calculated using ab initio coupled cluster and hybrid density functional methods with large basis sets up to the augmented correlation-consistent polarized quadruple-zeta (aug-cc-pVQZ) level. The effect of systematic basis set expansion on the calculated EA of CH_2Br and inversion barrier of CH_2Br^- has been investigated with the two theoretical approaches. Electron localization function (ELF) topological analysis of the $\text{CH}_2\text{Br}/\text{CH}_2\text{Br}^-$ system is performed to enlighten the process of electron attachment to CH_2Br to form CH_2Br^- .

Adres publiczny

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