AB INITIO VIBRATIONAL ANALYSIS OF 3,3-DIMETHYL-1-(TRIMETHYLPLUMBYL)CYCLOPROPENE

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The geometrical parameters and quantum-chemical force fields for 3,3-dimethylcyclopropene and its 1-(trimethylX) derivatives (X = C, Si, Ge, Sn, or Pb) were calculated at the pseudopotential (HF/SDDAll) level. The set of scale factors for correction of these force fields was determined using the well-characterized vibrational spectrum of derivative with X = Si. Transferral of the set of scale factors obtained to all these molecules was followed by calculation of their vibrational wavenumbers. Analysis of the results obtained revealed some peculiarities in the vibrational wavenumbers of these molecules [1].

Литература

1. G.R. De Maré, Yu.N. Panchenko, A.V. Abramenkov, Spectrochim. Acta, 67A (2007) 1094-1100.