SECONDARY PERIODICITY IN THE STRUCTURAL AND VIBRATIONAL CHARACTERISTICS OF 3,3-DIMETHYLCYCLOPROPENES DI- AND MONOSUBSTITUTED BY $-X(CH_3)_3$ (X = C, Si, Ge, Sn, Pb)

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The regularities of changes in the structural parameters and vibrational wavenumbers have been traced for certain moieties of the title compounds. The optimized geometrical parameters and the force fields of disubstituted 3,3-dimethylcyclopropenes[a] and monosubstituted 3,3-dimethylcyclopropenes[b] were determined at the HF/3-21G* and DDAll levels, respectively. The choice of these theoretical levels was brought about by peculiarities of GAUSSIAN 03 suite of programs for Sn and Pb atoms. The theoretical vibrational wavenumbers were calculated from the corresponding scaled force fields. The regularities obtained in the form of the zigzag lines are analogous to regularities that are characteristic to the atoms of the 14 (IVA) group of the Mendeleyev Periodic Table. This is known as the secondary periodicity phenomenon.

[a] Yu. N. Panchenko, G. R. De Maré, A. V. Abramenkov, and A. de Meijere, *Spectrochim. Acta* 65A, 575 (2006).
[b] G. R. De Maré, Yu. N. Panchenko, and A. V. Abramenkov, *Spectrochim. Acta* 67A, 1094 (2007).