L05. Molecular structure and IR spectra of phosphorus dendrimers by DFT calculations

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The main features of vibrational spectra of starburst dendrimers have been analysed for the first time. Their spectral pattern, in general, is determined by the ratio of a number of terminal groups to a number of repeating units. This ratio trends to mr – 1 (mr – branching functionality of repeating unit), and become the constant, when generation number of the starburst dendrimer increases higher than 3-5. IR and Raman spectra of the twelve generations of the phosphorus-containing dendrimers are represented and interpreted on the basis of the calculation of frequencies of the normal vibrations and band intensities in the IR spectra of terminated by dangling methyl groups "molecules", which are the fragments of dendrimer molecule. Tailored spectra of these fragments then compared with experimental spectra and satisfactory similarity have been obtained. Experimental spectra of generations higher than 4 are very close similar, ac-cording theoretical approach. The results can be used for the analysis of the chemical and physical transformations in starburst dendrimers.