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Vibrational spectroscopic study of cationic phosphorus dendrimers with aminoethylpiperidine terminal groups

V.L. Furer[a,*], A.E. Vandyukov[b], V. Tripathi[c], J.P. Majoral[c], A.M. Caminade[c], V.I. Kovalenko[b,d**]

[a]*Kazan State Architect and Civil Engineering University, Zelenaya, 1, Kazan 420043, Russia*

[b]*A.E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Science, Arbuzov Str., 8, Kazan 420088, Russia*

[c]*Laboratoire de Chimie de Coordination, CNRS, 205 route de Narbonne, 31077 Toulouse Cedex 4, France*

[d] *Kazan National Research Technological University, 68, Karl Marx Str., Kazan 420015, Russia*

Abstract

Two generations of phosphoric dendrimers with piperidine functional groups were synthesized for use in biology and medicine. Neutral samples are soluble in organic solvents but after protonation these dendrimers become water soluble and can be used for biological experiments. The FTIR and FT Raman spectra of two generations of dendrimers G_i constructed from the cyclotriphosphazene core, repeating units **–O–C_6H_4–CH=N–$N(CH_3)$–P(S)<** and aminoethylpiperidine end groups **–NH–$(CH_2)_2$–C_5NH_{11}** were recorded. The study of the IR spectra shows that the NH groups form hydrogen bonds. The calculation of the molecular structure and vibrational spectra of the first generation dendrimer was performed by the method of DFT. This molecule has flat, repeating units and a plane of symmetry passing through the core. The calculation of the distribution of potential energy made it possible to classify the bands in the experimental spectra of dendrimers. Amine groups are manifested in the form of a band of NH stretching vibrations at 3389 cm^{-1} in the IR spectrum of G_1. NH^+ stretching bands located at 2646 and 2540 cm^{-1} in the IR spectrum of G_2. The stretching vibrations of NH^+ groups are noticeably shifted to low frequencies due to the formation of a hydrogen bond with the chlorine atom. The line at 1575 cm^{-1} in the Raman spectrum of G_1 is characteristic for repeating units.

Keywords: Dendrimers, Raman spectra, IR spectra, Normal vibrations, DFT

* Tel.: +7-8432-104737; fax.: +7-8432-387972. E-mail address: furer@kgasu.ru (V.L. Furer).
*Tel.: +7-8432-732283; fax.: +7-8432-732253. E-mail address: koval@iopc.ru (V.I. Kovalenko).