Structure, IR and Raman Spectra of the *N*-[4-(Octan-2-Yloxy)Benzyl]-*N*,*N*-Dimethyl-Hexadecane-1-Aminium Molecule – Promising Object for Liquid Crystal Systems

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The *N*-[4-(Octan-2-Yloxy)Benzyl]-*N*,*N*-Dimethyl-Hexadecane-1-Aminium (N4OYBDHA) molecule contains 97 atoms: 62 hydrogen atoms, 33 carbon atoms, 1 nitrogen, and 1 oxygen atoms. Since the N4OYBDHA molecule contains many atoms, the finding of its equilibrium configuration was carried out in several stages. First of all the molecular geometry was optimized at the HF/cc-pVDZ level of theory. Then optimized geometrical parameters were used for finding equilibrium configuration at the B3LYP/cc-pVDZ level of theory. At the last stage, these optimized parameters were used for geometry optimization at the B3LYP/cc-pVTZ level of theory. The equilibrium geometry of the N4OYBDHA molecule is shown in Fig. 1.

Fig. 1. Equilibrium configuration of the N4OYBDHA molecule calculated at the B3LYP/cc-pVTZ level of theory.

According to calculations, the longitudinal and transverse dimensions of the molecule turn out to be 36 and 7 Å, respectively. The value of the dipole moment is 12.9 Debye and it is directed along with the carbon skeleton of the molecule. Using equilibrium geometry of the molecule IR and Raman spectra were calculated at the B3LYP/cc-pVTZ level of theory. Due to N4OYBDHA molecule contains 21 methylene (CH_2) groups the large number from the 285 normal modes are a) scissoring, twisting, wagging, and rocking vibrations of these groups as well as b) stretching vibrations of the C-C and C-H bonds. However, most of the a) types vibrations produced very weak IR bands and Raman lines. Most intensive expected bands and lines in the IR and Raman spectra of the N4OYBDHA were analyzed too.