

# Quantum chemistry modeling of cyclophosphazenes derivatives and their supramolecular complexes

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The structure-properties correlation is the main purpose of present investigation. Particularly, self-assembling multifunctional inorganic/organic building blocks on the cyclophosphazene basis were studied with previous computation and computer modeling. At the first time quantum chemistry analysis was applied both to supramolecular assembles for small initial cyclophosphazenes  $P_nN_nCl_{2n}$  ( $n = 2,3,4,5,6$ ) molecules and to their biopolymer derivatives with spacer groups  $-O(C_6H_4)NH_2$ ,  $-NH(C_6H_4)COOH$ - and others. Quantum-chemical calculation permits to predict different structures using electron density value, electronic laplacian for definition of electron localization function.

Hexaarms biopolymers with cyclophosphazene skeleton was obtained and identified. The ordered  $\alpha$ -helical conformation in transconfiguration was shown by Fourier transform infrared (FT-IR) spectroscopy and nuclear magnetic resonance (NMR) data. Computer modeling of optimized structures demonstrates unusual assembles of arched form with regular order inside every chain and several cavities inside bundles. Cambridge Date Base was used for building of initial models.

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