



**Заключителна конференция по проект „МАДАРА”:
ИЗЧИСЛИТЕЛЕН КОМПЛЕКС ЗА АВАНГАРДНИ ИЗСЛЕДВАНИЯ ПО
МОЛЕКУЛЕН ДИЗАЙН, НОВИ МАТЕРИАЛИ И НАНОТЕХНОЛОГИИ**

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СОФИЯ, БЪЛГАРИЯ

РЕЗЮМЕТА

на докладите

Tacticity of poly(butyl- α -cyanoacrylate) chains in nanoparticles: NMR spectroscopy and DFT calculations

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NMR spectroscopy and quantum chemical calculations were applied for structural characterization and determination of the preferred stereochemical sequence distribution of the monomer units in the homopolymer chains of poly(butyl- α -cyanoacrylate) nanoparticles. The stereochemical sequence distribution of the monomer units was defined by analysis of their high-resolution 1D ^1H and ^{13}C NMR and 2D J-resolved, $^1\text{H}/^{13}\text{C}$ HSQC and $^1\text{H}/^{13}\text{C}$ HMBC NMR spectra. The results were verified by employment of B3LYP/6-31G(d) calculations and are consistent with the preferred tendency of polymer chains of PBCN to adopt syndiotactic placements. The proton and carbon chemical shielding were calculated at BPW91/6-31+G(d) level using the GIAO approach and B3LYP/6-31G(d) optimized geometry.

