

Rationally designed octa-imine silsesquioxanes: Insights into structural and thermal properties

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Streszczenie

Polyhedral oligomeric silsesquioxanes (POSS) are increasingly recognized as versatile hybrid organic–inorganic materials, attributed to their well-defined nanocage architectures, customizable functionalities, and exceptional thermal stability. This study report the synthesis, structural characterization, and thermal analysis of a novel series of octa-substituted imine-functionalized POSS derivatives, featuring hydroxyphenyl, bromophenyl, thiophene, and dibenzofuran groups. Comprehensive spectroscopic analyses—including ^1H , ^{13}C , and ^{29}Si NMR, diffuse reflectance infrared Fourier transform spectroscopy (DRIFT), and UV-Vis spectroscopy—alongside high-resolution mass spectrometry and single-crystal X-ray diffraction, confirmed complete octa-substitution and the integrity of the T_8 siloxane cage. Structural investigations revealed the presence of non-covalent interactions that shape the supramolecular organization of these compounds. Thermogravimetric analysis (TGA) demonstrated high decomposition temperatures (305–326 °C) and ceramic yields aligning with theoretical SiO_2 formation. The diverse structural motifs and tunable properties of these imine-functionalized POSS derivatives highlight their potential utility in areas such as porous materials, green catalysis, and molecular electronics.

Słowa kluczowe

Polyhedral oligomeric silsesquioxanes (POSS), Nanocage architectures, Singlecrystal X-ray diffraction, Thermogravimetric analysis (TGA), Imine-functionalized POSS, Non-covalent Interaction

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