

Coordination polymers containing

1,3-Phenylenebis-((1H-1,2,4-triazol-1-yl)methanone) ligand: Synthesis and ϵ -caprolactone polymerization behavior

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The reaction of isophthaloyl dichloride with 1H-1,2,4-triazole afforded the new ligand 1,3-phenylenebis(1,2,4-triazole-1-yl)methanone (1). A series of Co(II), Cu(II), Zn(II) and Ni(II) complexes were synthesized using 1 and then characterized by melting point analysis, elemental analysis, theoretical calculations, thermogravimetric analysis, X-ray powder diffraction, nuclear magnetic resonance, infrared and Raman spectroscopy. Experimental and computational studies predict the formation of coordination polymers (CPs). The cobalt and copper CPs and zinc(II) complex were found to be good initiators for the ring-opening polymerization of ϵ -caprolactone (CL) under solvent-free conditions. ¹H-NMR analysis showed that the obtained polymers of CL were mainly linear and had terminal hydroxymethylene groups. Differential scanning calorimetry showed that the obtained polycaprolactones had high crystallinity, and TGA showed that they had decomposition temperatures above 400 C. These results provide insight and guidance for the design of metal complexes with potential applications in the polymerization of CL. © 2017 by the authors.

ϵ -Caprolactone Polymerization

Coordination Polymers

Initiators

Triazole Ligand

caprolactone

coordination compound

hexanoic acid derivative

lactone

ligand

polymer

triazole derivative

chemistry

computer simulation

infrared spectrophotometry

molecular model

polymerization

synthesis

thermogravimetry

X ray diffraction

Caproates

Computer Simulation

Coordination Complexes

Lactones

Ligands

Models, Molecular

Polymerization

Polymers

Spectrophotometry, Infrared

Thermogravimetry

Triazoles

X-Ray Diffraction