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Nontemplate synthesis, characterization and theoretical study of tetraazamacrocycles

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Abstract The syntheses of new tetraaza macrocyclic compounds of variable ring sizes by non-template methods and their characterization with the help of elemental analysis and spectroscopic techniques (FT-IR, ^{1}H-NMR, and ^{13}C-NMR) have been reported in detail. The vibrational frequencies determined experimentally are compared with those obtained theoretically from density functional theory (DFT) and Hartree-Fock (HF) calculations. The comparisons between the experimental and theoretical results indicate that B3LYP level with both the 3-21G(d) and 6-31G+(d,p) basis sets is able to provide satisfactory results for predicting IR properties. The frontier molecular orbital diagrams and molecular electrostatic potential maps of title compounds have been also calculated and visualized at the B3LYP/6-31G+(d,p) level of theory.

Keywords: Macrocyclic ligands, Computational methods, DFT, HF, ab-initio

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