Template synthesis of two new supramolecular zinc(II) complexes containing pentadentate N₃O₂ semicarbazone ligand: Nanostructure synthesis, Hirshfeld surface analysis, and DFT studies

Yunes Abbasi Tyula a, Abedien Zabardasti a, *, Hamid Goudarziafshar b, Majid Sadeghi Roudsari c, Michal Dusek d, Vaclav Eigner d

a Department of Chemistry, Lorestan University, Khorramabad, Iran
b Department of Chemistry, Faculty of Science Saeed Jameleddinmasadabadi University, Asadabad, Iran
c Department of Inorganic Chemistry, Faculty of Chemistry, Tabriz University, 51666-14766, Tabriz, Iran
d Institute of Physics of ASCR, v.v.i, Na Slovance 2, 18221, Prague 8, Czech Republic

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1. Introduction

In recent decades, the design and synthesis of supramolecular coordination compounds have attracted considerable interest due to their potential applications in various fields such as catalysis, anticancer agents, gas storage, magnetism, luminescence, nonlinear optics and molecular sensing [1–6]. Different factors can be involved in designing supramolecular compounds such as coordination bonding interactions, relatively strong hydrogen bonding, and π–π stacking interactions, ligand geometry, solvent molecules, counter ions and metal ions and the reaction conditions [7–10]. Flexible isonicotinyl hydrazide Schiff base ligands (hydrazones, R-CO-NH–N=CH-R′) and their derivatives with multifarious coordination modes are good candidates to produce supramolecular structures [11,12], because they often acting as chelating/bridging ligands through their N and O atoms [13–16], and also the aromatic portion of these ligands are good candidates for spacer part of organic-inorganic materials, because not merely they can act as hydrogen-bonding acceptors or donors, but can also provide identification sites for π–π stacking interactions to form attractive supramolecular structures when coordinating to metal centers. Moreover, hydrazones and their coordination complexes are an interesting class of compounds which possess various applications such as molecular sensors [17], catalysts [18], magnetic properties [19], and a wide spectrum of biological activities (antimicrobial [20,21], anti-inflammatory [22], anticonvulsant [23], and anticancer [24]). On the other hand, 2,6-diacetylpyridine is an excellent precursor for synthesizing hydrazone Schiff bases which usually act as planar pentadentate ligands in creating pentagonal-

* Corresponding author.
E-mail addresses: zebardasti@yahoo.com (A. Zabardasti), majidsadeghi.chemi@yahoo.com (M.S. Roudsari), dusek@fzu.cz (M. Dusek), eigner@fzu.cz (V. Eigner).

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