

Mn(II)-mediated in situ cyclization of amino functionalized pyridine (iso)nicotinoyl-hydrazones into dipyridyltriazoles: One-pot route to supramolecular Mn(II)-complexes

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Rok wydania

2026

Czasopismo

Inorganica Chimica Acta

Numer woluminu

592

Strony

123033/1-123033/11

DOI

10.1016/j.ica.2025.123033

Kolekcja

Naukowa

Język

Angielski

Streszczenie

The development of efficient one-pot methodologies for the *in situ* construction of polydentate N-heterocyclic ligands and their integration into coordination frameworks remains a central challenge in synthetic inorganic chemistry. Herein, we report a one-pot reaction of amino-functionalized pyridine (iso)nicotinoyl hydrazones, thiocyanate, and Mn(II) salts in acetonitrile, which yields two new mixed-ligand Mn(II) coordination complexes, $[\text{Mn}(\text{HL}^3)_2(\text{NCS})_2(\text{H}_2\text{O})_2]$ (**1**) and $[\text{Mn}(\text{HL}^4)_4(\text{NCS})_2] \cdot \text{CH}_3\text{CN} \cdot 0.5(\text{H}_2\text{O})$ (**2**), where HL^3 and HL^4 represents two *in situ* formed dipyridyl-1H-1,2,4-triazole ligands. These ligands are formed through a Mn(II)-assisted cyclization of amino-functionalized pyridine (iso)nicotinoyl hydrazone precursors (HL^1 and HL^2 in acetonitrile). Single-crystal X-ray diffraction confirms the *in situ* ligand transformation and reveals that both complexes contain six-coordinate Mn(II) centers in distorted octahedral environments, extended through diverse noncovalent interactions into higher-dimensional frameworks. Furthermore, the electronic properties of both complexes **1** and **2** have been demonstrated through theoretical studies based on DFT calculations. Molecular packings of both complexes **1** and **2** show similarity for the first five levels of intermolecular interaction strength. Mechanistically, this work demonstrates the dual catalytic and template roles of Mn(II) in directing both ligand evolution and supramolecular architecture. Overall, this work presents a practical and generalizable strategy for the one-pot synthesis of adaptive coordination materials *via* metal-mediated heterocycle construction, contributing to ongoing advances in crystal engineering and supramolecular design.

Słowa kluczowe

(iso)nicotinoyl-hydrazones, Mn(II) complex, Single crystal, DFT, Topological analysis

Typ publikacji

Artykuł

Adres publiczny

<http://dx.doi.org/10.1016/j.ica.2025.123033>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-10-03 13:35:45

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/MjyFp7>.