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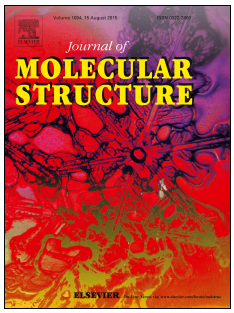

Synthesis, spectral and crystallographic study, DNA binding and molecular docking studies of homo dinuclear Co(II) and Ni(II) complexes

M. Shahnawaz Khan, Mohd Khalid, M. Shahwaz Ahmad, Musheer Ahmad, Mo Ashafaq, Rahisuddin, Rizwan Arif, M. Shahid

PII: S0022-2860(18)31003-2

DOI: 10.1016/j.molstruc.2018.08.048

Reference: MOLSTR 25569

To appear in: *Journal of Molecular Structure*

Received Date: 27 July 2018

Revised Date: 13 August 2018

Accepted Date: 16 August 2018

Please cite this article as: M.S. Khan, M. Khalid, M.S. Ahmad, M. Ahmad, M. Ashafaq, Rahisuddin, R. Arif, M. Shahid, Synthesis, spectral and crystallographic study, DNA binding and molecular docking studies of homo dinuclear Co(II) and Ni(II) complexes, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.08.048.

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Synthesis, spectral and crystallographic study, DNA binding and molecular docking studies of homo dinuclear Co(II) and Ni(II) complexes

M. Shahnawaz Khan[a], Mohd Khalid[a], M. Shahwaz Ahmad[a], Musheer Ahmad[b], Mo Ashafaq[a], Rahisuddin[c], Rizwan Arif[c], M. Shahid[a]*

[a]Department of Chemistry, Aligarh Muslim University, Aligarh 202002

[b]Department of Applied Chemistry, Aligarh Muslim University, Aligarh 202002

[c]Department of Chemistry, Jamia Millia Islamia, New Delhi

**Corresponding author, Email: khalid215@gmail.com*

Abstract

Two homo dinuclear metal complexes with composition $[M_2(pda)_2(H_2O)_5]\cdot 2H_2O$ (M= Ni^{2+} and Co^{2+}) have been synthesized and characterized by elemental, spectral and thermal analysis (UV-vis, FT-IR, Fluorescence, EPR, and TGA).The structures of complexes **1** and **2** have been determined by single crystal X-ray diffraction studies and the geometry around M(II) ion was elongated distorted octahedral. Binding studies of the complexes **1** and **2** with Ct-DNA was investigated by absorption, fluorescence and viscosity measurements. The experimental results of DNA binding studies were supported by theoretical (molecular docking analysis). DNA binding results reveal that complexes **1** and **2** binds to the minor groove of DNA and are stabilized through hydrogen bonding interactions.

Keywords: Homodinuclear complexes, Crystal structure, DNA binding, Molecular docking.

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