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REGULAR ARTICLE

Polymorph of *trans*-dichlorotetrakis(pyridine-*N*)ruthenium(II) influenced by a dihydrazone: crystal structure, spectral, Hirshfeld surfaces, antimicrobial, toxicity and *in silico* docking studies

DEBAJANI BASUMATARY[a,*], MADAN KUMAR SHANKAR[b], KULLAIAH BYRAPPA[c], KANDARPA KUMAR SAIKIA[d], AJAZ AHMAD DAR[e], VEDANT VIKROM BORAH[d], PRANJIT SARMA[a], PRANAMI MAHANTA[a], MRITUNJAYA ASTHANA[f] and NAMRATHA KEERTHIRAJ[g]

[a]Department of Applied Sciences, Gauhati University, Guwahati 781 014, India
[b]Institution of Excellence, Vijnana Bhavan, University of Mysore, Mysuru 570 006, India
[c]Research and Innovations Center, Adichunchanagiri University, B.G. Nagara, Mandya 571 448, India
[d]Department of Bioengineering and Technology, Gauhati University, Guwahati 781 014, India
[e]Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781 039, India
[f]TCG Lifesciences Pvt. Ltd, Salt Lake, Kolkata 700 091, India
[g]Department of Studies in Earth Science, Manasa Gangotri, University of Mysore, Mysuru 570 006, India
E-mail: debbasumatary@gmail.com; debbasumatary@gauhati.ac.in

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Abstract. Many reports describe the influence of additives or impurities on the physicochemical properties of crystals. On having obtained *trans*-[$RuCl_2(C_5H_5N)_4$] as brown, needle-shaped crystals contrary to red or orange-red blocks reported previously, we herein revisit its study. This complex was obtained from the filtrate of an ensuing reaction mixture of $RuCl_3{\cdot}3H_2O$, bis(2-hydroxy-l-naphthaldehyde)adipoyldihydrazone ($npahH_4$) and pyridine in methanol. Findings from X-ray crystallographic data and spectra of IR, UV-Visible, ^1H and ^{13}C NMR along with other analytical studies of the complex are presented here. A comparative study with previously reported crystal forms was performed to understand the accompanying molecular structural differences in the physical (shape, size and color) morphological alteration. Further probing into molecular dynamics, the molecular interactions were analyzed and quantified using computational methods. The symmetry of intermolecular interaction in C—H···Cl is different from earlier reported crystal forms. The intercontact H···H showed a major contribution (62.9%) for Hirshfeld surfaces. Also, we report antibacterial activity of the complex against methicillin-resistant *Staphylococcus aureus* followed by the *in silico* docking study that revealed its interaction with the residue Glu58 of ATPase subunit of *S. aureus* GyrB. Additional studies on its toxicity using rat models revealed this complex as non-toxic to animals.

Keywords. Crystal-color morphology; characterization; packing interactions; additive.

1. Introduction

The changes in physical characteristics of a crystal due to additives, impurities, solvent, supersaturation, polymorphism, etc., have been a subject of significant interest and extensive study.[1–9] The physical morphological differences may have an immense impact on the crystal properties like stability, solubility, packing, compaction, mechanical, chemical, electrical, etc.,[2,3] thus, altering the compound's characteristics. So certainly, the physical morphological variations can pave a way to change the compounds behavior for functional applications, such as for designing drugs and materials with desired characteristics.[10] However, crystallization being a complex phenomenon, the current understanding of its underlying mechanism is still rudimentary. There are many reports in the literature that have described the presence of additives or

*For correspondence

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