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

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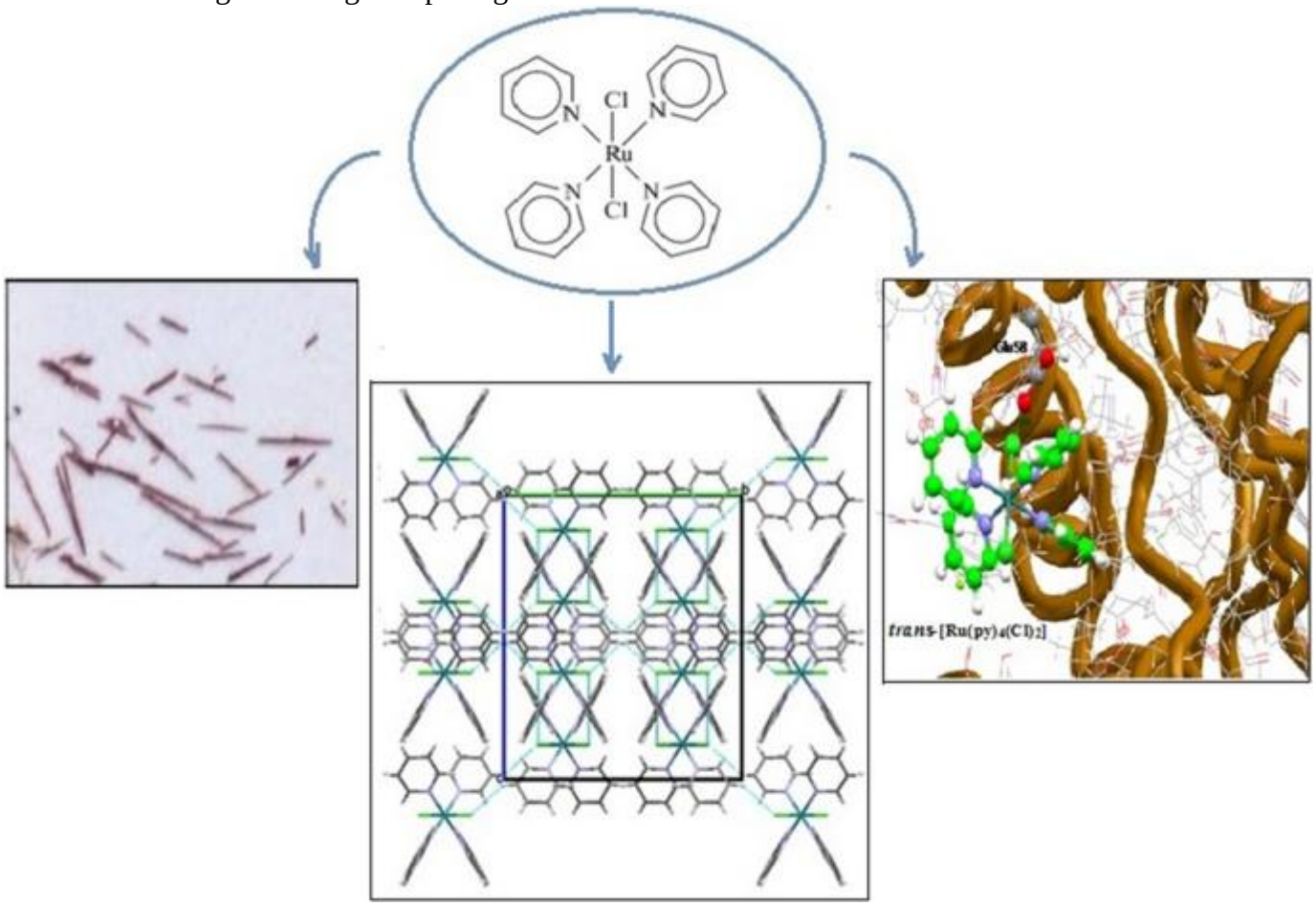
## Abstract

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, $^{1}H$ 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.

## Graphic abstract

**Synopsis**: The crystal and colour morphology of a polymorph of *trans*-[$RuCl_2(py)_4$] have been studied by different investigations. The intercontacts have been discussed. The significant influence of a dihydrazone in morphological changes is revealed. The biological aspects have been further investigated through non-toxicity, antimicrobial screening and molecular docking studies against pathogen *S. aureus*.



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