

# Synthesis, characterization, thermal aspects, density functional theory study and *in vitro* antibacterial evaluation of Cr(III) complexes based on pyrazolone phenylhydrazone ligands

Chintan P Somaiya<sup>\*a</sup>, Dinesh S Patel<sup>b</sup>, Darshan H Jani<sup>c</sup> & Drashti R Thanki<sup>a</sup>

<sup>a</sup>Department of Chemical Science, Parul Institute of Applied Sciences, Parul University, Vadodara 391 760, Gujarat, India

<sup>b</sup>Shree P. M. Patel Institute of Post Graduate Studies and Research in Science  
(Recognized Research Center of Sardar Patel University, V.V. Nagar) Anand 388 001, Gujarat, India

<sup>c</sup>Department of Chemistry, Faculty of Science, Noble University, Bhesan Road Bamangam, Junagadh 362 310, Gujarat, India

E- mail: somaiyachintan11@gmail.com

Received 23 July 2024; accepted(revised) 20 September 2024

This study examines the synthesis, characterization, computational analysis, and antibacterial activity of chromium (III) complexes with pyrazolone phenylhydrazone ligands. The ligands and their chromium (III) complexes have been synthesized and confirmed using various analytical techniques such as <sup>1</sup>H and <sup>13</sup>C NMR, mass spectrometry, elemental analysis, infrared spectroscopy, and UV-visible spectroscopy. The characterization of chromium (III) complexes involves elemental analysis, thermogravimetric analysis (TGA/DTG), differential scanning calorimetry (DSC), FAB mass spectrometry, and UV-visible spectroscopy, which validated their structures and properties. Additionally, the electronic properties and reactivity of the ligands and complexes have been investigated using DFT with the B3LYP/6-31G(d, p) basis set. The antimicrobial efficacy of the ligands and complexes have been tested against Gram-positive and Gram-negative bacteria, revealing significant antibacterial potential. These findings highlight the importance of pyrazolone phenylhydrazone-based chromium (III) complexes and suggest further exploration of their antimicrobial properties.

**Keywords:** 4-Acyl pyrazolone, Phenylhydrazone, Schiff base, Transition metal complex, DFT study, Antimicrobial activity