

## Synthesis, Investigation, DFT Study and Biologically Activity of Zirconium (IV) Complexes with Diammine Complexes

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**Abstract :** Zirconium diammin and triammin complexes can be possess biological activities, these complexes were synthesized via the reaction equimolar quantity of (1:10-phenanthroline){NC<sub>3</sub>H<sub>3</sub>(C<sub>6</sub>H<sub>2</sub>)NC<sub>3</sub>H<sub>3</sub>} (L1) or 4-4-amino phenazone {ONC<sub>6</sub>H<sub>5</sub>(NH)CH(NH<sub>2</sub>)} (L2) or diphenyl carbizon {HNCO(NH)<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>)} (L3) with Zirconium Salt {ZrOCl<sub>2</sub>} in ratio (1:1) to form complexes [{NC<sub>3</sub>H<sub>3</sub>(C<sub>6</sub>H<sub>2</sub>)NC<sub>3</sub>H<sub>3</sub>}ZrOCl<sub>2</sub>] [ZrOCl<sub>2</sub>L<sub>1</sub>], [{(O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>(NH)(NH<sub>2</sub>))ZrOCl<sub>2</sub>] [ZrOCl<sub>2</sub>L<sub>2</sub>] and [{HNCO(NH)<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>)ZrOCl<sub>2</sub>] [ZrOCl<sub>2</sub>L<sub>3</sub>] respectively. The characterization of these complexes were follow by using Fourier Transform Infrared (FT-IR) and UV-Visible spectroscopy. Also a variable temperature study of these complexes has been followed by using UV-Visible spectroscopy to follow electronic transform behaviors under temperature control also DFT study calculation was follow these complexes via the information from FT-IR and UV-Visible spectroscopy. A coordination number of these complexes of types five and six of the geometry can be suggested. These complexes were found to shown deferent inhibition to the growth of bacterial strains of Bacillus spp & Klebsiella spp & E.coli & proteus spp & pseudomona spp) while all complexes were in deferent's concentration (0.001, 0.2 and 1M) and the result as evidenced from the presence. For better understanding these complexes were examined by using Density functional theory (DFT) calculation.

**Keywords :** (1:10-phenanthroline) (L1), 4-4-amino phenazone (L2), diphenyl carbizon (L3), DFT study, antibacterial

**Conference Title :** ICSRD 2020 : International Conference on Scientific Research and Development

**Conference Location :** Chicago, United States

**Conference Dates :** December 12-13, 2020