



SDI FINAL EVALUATION FORM 1.1

PART 1:

Journal Name:	American Chemical Science Journal
Manuscript Number:	2014_ACSj_10427
Title of the Manuscript:	Stability and Antimicrobial Activity of Transition Metal(II) Complexes with SNO and ONO Functionalized Ligand: A Computational Study

PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	Authors' response to final evaluator's comments
IR Spectra: Add the discussion about metal to ligand stretching bands like M-N, M-O and M-X stretching bands you observed in all complexes' IR spectra differ from the respective ligands' IR spectra. Electronic Spectra: Authors have to add some stuffs about d-d transition of all complexes as they had prepared the transition metal complexes from the ligands. Mass Spectra: Discuss some fragmentations and peak pattern you observed in ligands' mass spectra and complexes' mass spectra. Is there any coordinated or lattice water molecules present in your complexes?	** I should bring to your attention that the main concern of our work is computational, where the access to experimental resources in our institution is limited. However, please consider the following notes: - IR Spectra: IR was employed for each of our complex in 4000–400 cm^{-1} range. Obvious new bands at 455 cm^{-1} (which already listed in the experimental part) could be assigned to the respective (M-O) frequencies. However, expected at the end of the scale (410 cm^{-1}), the (M-N) band has not been detected. Also, expected at frequency lower than 400 cm^{-1}, (M-S) bands could not be observed. - Electronic Spectra: Commonly, Zinc complexes with d^{10} electronic configuration, have no allowed d-d transition. Other complexes may show a d-d transition associated with weak and broad peak. However, in this study due to the intense absorption of charge transfer, bands associated with (d-d) bands were masked. [See: Housecroft, Sharpe, Inorganic Chemistry, 2ed ed, Pearson Prentice Hall, 2005, P. 570.) - Mass Spectra: The only fragment appears clearly corresponding to the ligand at 232 - There is no access to X-ray studies