

Vita

Candidate's name: Weihao Da

Universities
Attended: Changzhou University (2016)
Bachelor of Science

St. Francis Xavier University (2018)
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Masters of Science

Conference Presentations:

Da W., Blight B.*, Synthesis of thiourea and guanidine containing cobalt (II), rhodium (III), platinum (II) complexes, and binding studies of their second-sphere H-bonding host-guest system, 27th Annual UNB Graduate Research Conference 2021 (UNB GRC 2021).

Da W., Blight B.*, Synthesis of thiourea and guanidine containing cobalt (II), rhodium (III), platinum (II) complexes, and binding studies of their second-sphere H-bonding host-guest system, 2021 Royal Society of Chemistry Poster Twitter Conference

Synthesis of thiourea and guanidine containing cobalt (II), rhodium (III), platinum (II) complexes, and binding studies of their second-sphere H-bonding host-guest system

UNIVERSITY OF NEW BRUNSWICK
THESIS DEFENCE AND EXAMINATION

in Partial Fulfillment

of the Requirement for the Degree of
Master of Science

by

Weihao Da

in the Department of Chemistry

U.N.B., Fredericton, N.B.

Wednesday, August 25th, 2021
9:00 a.m.

Via MS TEAMS

Examining Committee

Dr. Barry Blight	Supervisor
Dr. Gilles Villemure	Internal Examiner
Dr. Amy Parachnowitsch	Int-Ext Examiner
Dr. Ghislain Deslongchamps	Chair of Oral Examination

Abstract

Supramolecular chemistry has seen a burgeoning interest over the last few decades for the fascinating findings that lie beyond the molecule. Supramolecular chemistry can also offer a fresh interface with biological and materials science. My research project is focused on designing, synthesizing, and exploring the intrinsic properties of complexes based on cobalt, rhodium, and platinum. In each case, thiourea/guanidine derivatives are our ligands of choice to confer H-bonding sites for second-sphere coordination of guest molecules. Second-sphere H-bonding interactions with three different guest molecules were analyzed to obtain association constants (K_a values) from $\sim 10^2 \text{ M}^{-1}$ to $\sim 10^4 \text{ M}^{-1}$ via UV-vis titration studies. Five sets of single crystal X-Ray diffraction data of our novel complexes were also acquired, alongside the result of a thermochromism test of one of our cobalt complexes. Obtained interesting features of our compounds include self-recognition and self-assembled structures. Overall, six novel thiourea/guanidine ligand-containing complexes – two for each of cobalt (II), rhodium (III) and platinum (II) - were synthesized. Through these dynamic H-bonding interactions, we see potential

applications of our molecules across the fields of medicine, biology, agriculture, and more. Our Host-Guest studies prove that these complexes are able to bind with DNA nucleobase-like molecules via hydrogen bonding, meaning that anticancer assays of our platinum (II) and rhodium (III) thiourea/guanidine-containing compounds are promising avenues for future evaluation. Results of dilution studies show potential supramolecular oligomer structures formed in dynamic system. Finally, testing our compounds within the arena of organometallic catalysis for specific reactions is also promising work that lies ahead.