Vita

Candidate's name: Jacob Miles Dore

Universities Attended: University of New Brunswick (2017)
Bachelor of Medicinal Chemistry

University of New Brunswick (2019)
Masters of Science

Publications/Conference Presentations:

J. M. Dore, A. G. Adam, D. W. Tokaryk, C. Linton, *Hyperfine analysis of the (2, 0) [18.3]3-$X^3\Delta_3$ transition of cobalt monoboride*, Journal of Molecular Spectroscopy, 360 (2019), 44-48

"Fine and Hyperfine Analysis of Ruthenium Monoboride Isotopologues." J. Dore, A. Adam, D. Tokaryk and C. Linton. 74th Meeting of the International Symposium on Molecular Spectroscopy, University of Illinois, Champaign-Urbana, June 2019 (talk).

"High Resolution Visible Spectroscopy of Ruthenium Monoboride." A. Adam, J. Dore, C. Linton, D. Tokaryk. 34th Meeting of the Symposium on Chemical Physics, University of Waterloo, Ontario, November 2018.

Laser-Induced Fluorescence Spectroscopy of Cobalt Monoboride and Ruthenium Monoboride

UNIVERSITY OF NEW BRUNSWICK

THESIS DEFENCE AND EXAMINATION

in Partial Fulfillment

of the Requirement for the Degree of
Master of Science

by

Jacob M. Dore

in the Department of Chemistry

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

Monday, July 22nd, 2019
10:00 a.m.

Toole Hall, Room 3

Examining Committee

Dr. Allan Adam	Supervisor
Dr. John Neville	Internal Examiner
Dr. Dennis Tokaryk	Int-Ext Examiner
Dr. Gilles Villemure	Chair of Oral Examination

Abstract

The electronic spectra of cobalt monoboride (CoB) and ruthenium monoboride (RuB) have been studied in the visible region of the electromagnetic spectrum. Both of these molecules have been previously studied by the Cheung group at medium resolution [1, 2]. In this thesis, the first high-resolution study performed on either molecule is reported. The previous spectroscopic study of CoB failed to resolve any hyperfine structure, and the work on RuB failed to resolve any of the ruthenium isotopes. The transition metal monoborides were produced in a laser ablation molecular jet apparatus and detected using laser-induced fluorescence (LIF) spectroscopy.

Fine and hyperfine interaction parameters in the [18.3]3 (v'=2) and $X^3\Delta_3$ (v''=0) states of CoB have been determined from an analysis of the high-resolution LIF spectrum. In this thesis, updated rotational parameters for both states of CoB are reported, as well as hyperfine interaction parameters arising from the strong nuclear interaction of ^{59}Co (I=7/2, μ/μ_N = 4.627) with the magnetic fields produced by the molecule. Atomic hyperfine calculations have been conducted and support the $X^3\Delta_3$ ground state and indicate that the excited [18.3]3 state is formed from a mixing of configurations but the biggest contribution coming from a $^3\Delta_3$ state.

The (1, 0), (0, 0) and (0, 1) bands of the [18.4]2.5-$X^2\Delta_{5/2}$ electronic transition of RuB have been taken with our high-resolution laser system. Ruthenium has 7 naturally occurring isotopes ranging from 1.87% - 31.55% abundance and boron has 2 (^{11}B: 80.1% and ^{10}B: 19.9%), giving a total combination of 14 isotopologues for RuB, of which we were able to isotopically analyze 12. Both of the odd isotopes of Ru have a nuclear spin I=5/2 and their respective isotopologues had resolved hyperfine structure which was analyzed to extract the hyperfine parameters. It was determined that the hyperfine interaction arises from the nuclear spin of the ^{101}Ru and ^{99}Ru atoms and not from the boron nucleus. Atomic hyperfine calculations have also been conducted for RuB and help support the ground state symmetry, $X^2\Delta_{5/2}$, and suggest that the likely contribution to the excited state is coming from a $^2\Phi_{5/2}$ state.