

Vita

Candidate's name: Madeleine Emerise Leger

Universities
Attended: University of Indianapolis (2019)
Bachelor of Science

University of New Brunswick (2021)
Masters of Science

Conference Presentations/Publications:

Poster: RSC Twitter Poster Competition 2021

Presentation: UNB Graduate Research Conference 2021

Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Hatem M. Titi, Tomislav Friščić, Barry A. Blight, and Bruce Balcom. "Relaxation Time Correlation NMR for Mechanochemical *in-situ* Reaction Monitoring of Metal-Organic Frameworks" doi.org/10.33774/CHEMRXIV-2021-RBJ0T. (submitted)

Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Tomislav Friščić, Bruce Balcom, and Barry A. Blight. "T₁-T₂* Relaxation Time Correlation NMR Monitoring of Mechano-Organic Reactions Forming Quinoxaline Derivatives" (in progress)

T₁-T₂* Relaxation Time Measurements to Monitor Mechanochemical Reactions

UNIVERSITY OF NEW BRUNSWICK
THESIS DEFENCE AND EXAMINATION
in Partial Fulfillment
of the Requirement for the Degree of
Master of Science

by

Madeleine E. Leger

in the Department of Chemistry

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

**Friday, December 17th, 2021
9:30 a.m.**

via MS TEAMS

Examining Committee

Dr. Barry Blight	Co-Supervisor
Dr. Bruce Balcom	Co-Supervisor
Dr. Larry Calhoun	Internal Examiner
Dr. Igor Mastikhin	Int-Ext Examiner
Dr. Gilles Villemure	Chair of Oral Examination

Abstract

Mechanochemistry has quickly grown into a popular field of chemistry because of its environmental benefits and its wide scope of chemical reactions and industrial applications. While the mechanisms are still poorly understood, many attempts have been made to better understand using *in-situ* and real-time measurements, such as Raman spectroscopy and synchrotron X-ray diffraction. Magnetic resonance is widely used across medical, industrial, and academic fields. Relaxation time correlation measurements are of interest for many samples and applications. Solid samples can be challenging to measure and have not often been analysed using relaxation time correlation measurements. Here, we employ ^1H T_1 - T_2^* correlation measurements to analyse and monitor mechanochemical reactions of quinoxaline derivatives and metal-organic frameworks (MOFs). With the MOF reactions, *in-situ* measurements were employed using lab-made Teflon jars.

Exponential and non-exponential data processing was compared and used to verify conservation of signal.