

The Use of ${}^6\text{Li}\{{}^7\text{Li}\}$ -REDOR NMR Spectroscopy to Compare the Ionic Conductivities of Solid-State Lithium Ion Electrolytes

T. L. Spencer^I, N. W. Plagos^I, D. H. Brouwer^{II}, G. R. Goward^{I*}

I. McMaster University, Department of Chemistry and Chemical Biology, 1280 Main St. West,
Hamilton, Ontario, Canada, L8S 1H2

II. Redeemer University College, Department of Chemistry, 777 Garner Road East, Ancaster,
ON, L9K 1J4

Supplementary Information

SPINEVOLUTION File for ${}^6\text{Li}\{{}^7\text{Li}\}$ -REDOR Curve Simulation

***** The System *****

spectrometer(MHz) 500

spinning_freq(kHz) 25

channels Li6(73.599 1) Li7

nuclei Li6 Li7

atomic_coords *

cs_isotropic 0 0

csa_parameters *

j_coupling Jiso2

quadrupole *

dip_switchboard *

csa_switchboard *

exchange_nuclei *

bond_len_nuclei *

bond_ang_nuclei *

tors_ang_nuclei *

groups_nuclei *

***** Pulse Sequence *****

CHN 1

timing(usec)	(40)128	38	2	40	(40)128
power(kHz)	0	0	250	0	0
phase(deg)	0	0	0	0	0
freq_offs(kHz)	0	0	0	0	0

CHN 2

timing(usec)	(redor-9.pp)	18	2	20	redor-9.pp	(redor-9.pp)
power(kHz)	*	0	250	0	*	*
phase(deg)	*	0	0	0	*	*
freq_offs(kHz)	*	0	0	0	*	*

***** Variables *****

wr=25

spinning_freq=wr

tr=1000/wr

***** Options *****

rho0 I1x

observables I1p

EulerAngles zcw987

n_gamma 10

line_broaden(Hz) *

zerofill *

FFT_dimensions *

options -dw123 -re

See another version of thhis input file in the
examples-new/dim-sections directory, and the
analytic mode version in examples-new/analyt

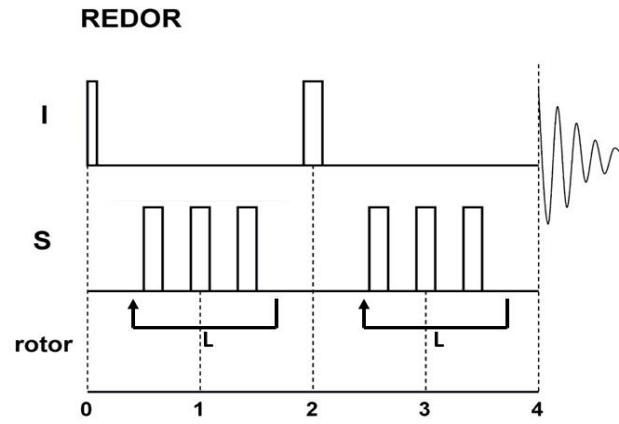


Figure S1. Rotational Echo Double Resonance (REDOR) pulse sequence. **I** and **S** represent two different spins, ${}^6\text{Li}$ and ${}^7\text{Li}$, respectively.

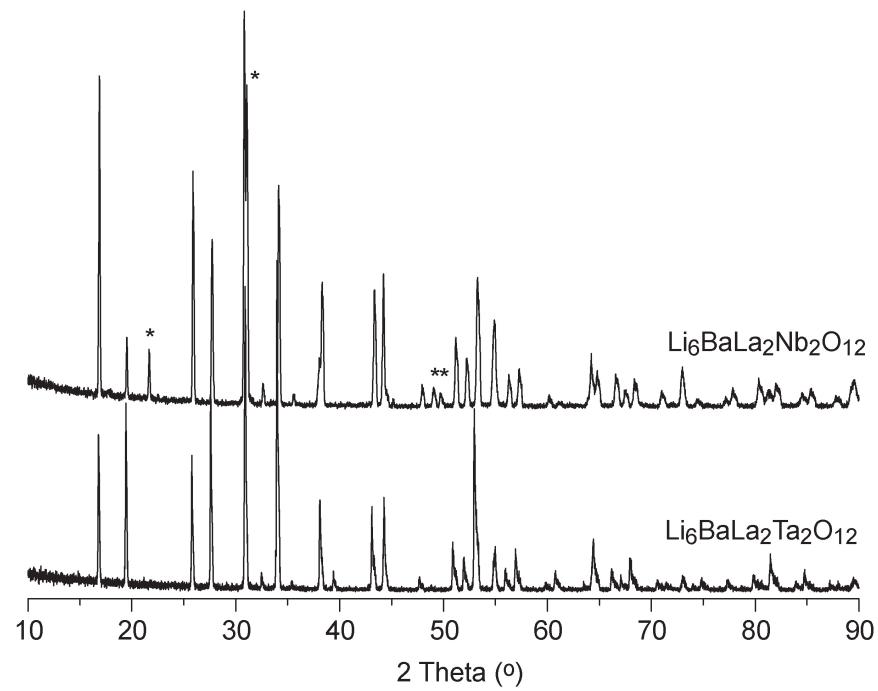


Figure S2. Powder X-ray diffraction patterns of ${}^{6,7}\text{Li}_6\text{BaLa}_2\text{Ta}_2\text{O}_{12}$ and the corresponding Nb phase. * represents an impurity phase.

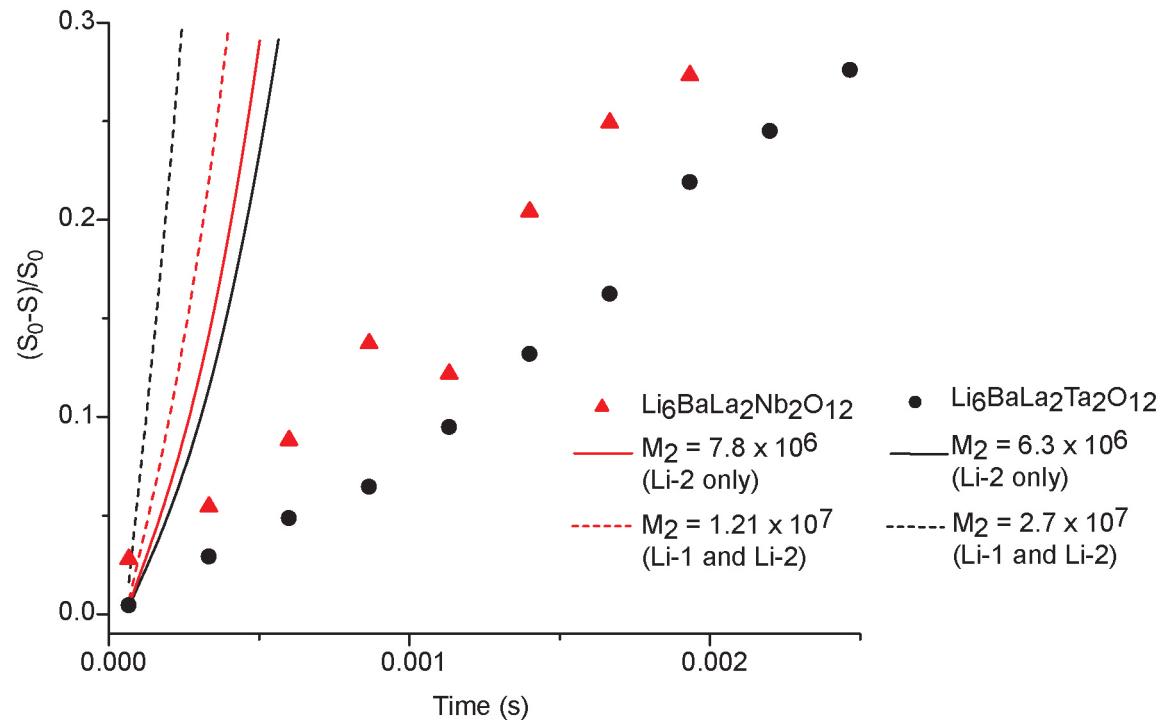


Figure S3. M_2 calculations for the Ta and Nb electrolyte phases using **Equation 5** for cases in which only Li-2 is occupied, and cases in which Li-1 and Li-2 are occupied in the model structure.