

Novel Electrolytes for use in Li-Air Batteries for NASA Electric Aircraft



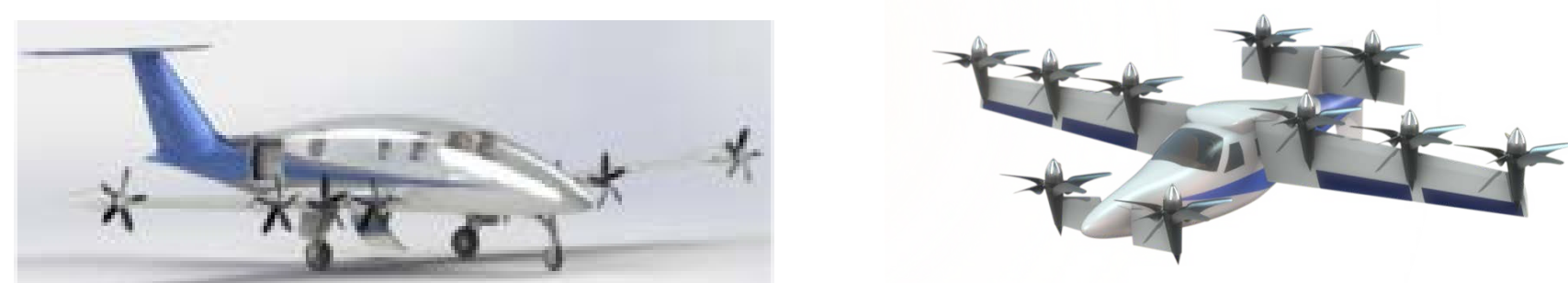
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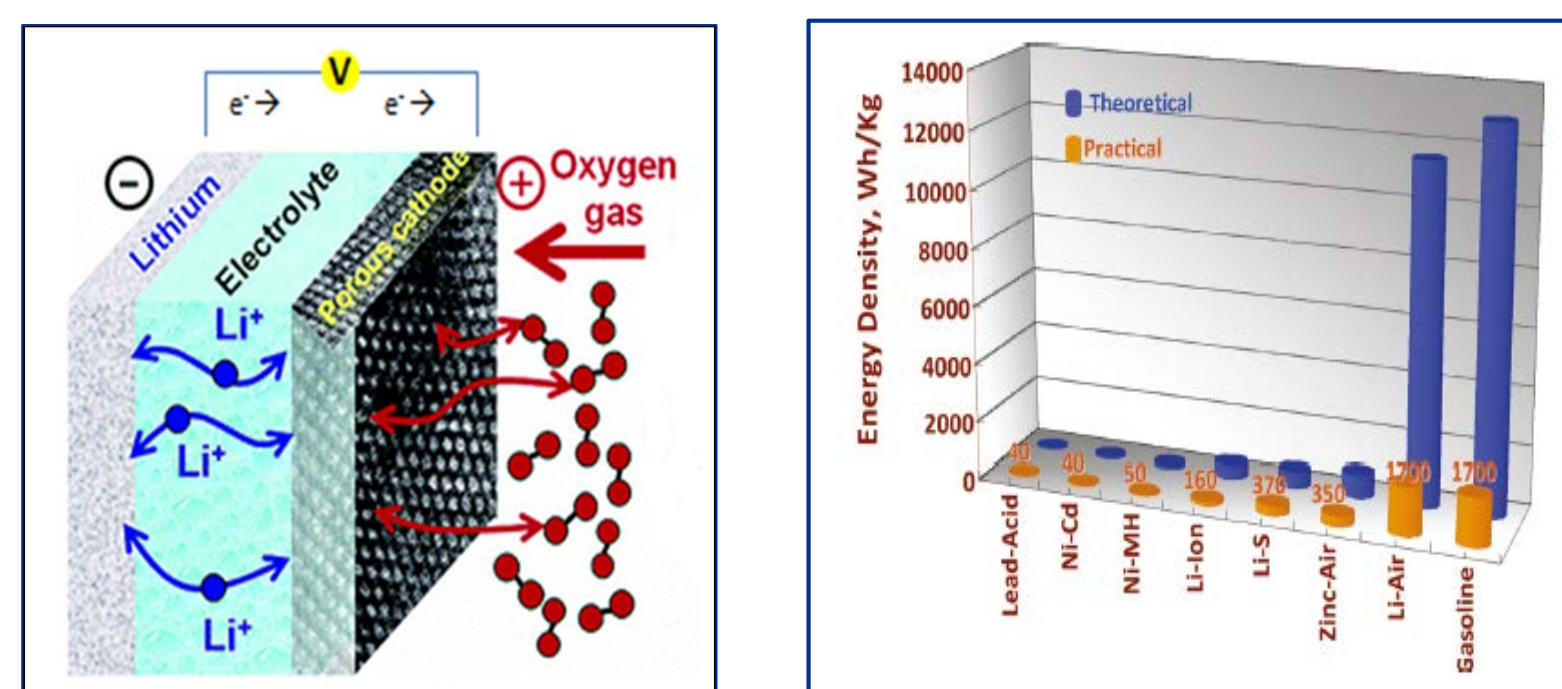
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Introduction

The 2018 Strategic Implementation Plan sets forth the NASA Aeronautics Research Mission Directorate (ARMD) vision for aeronautical research aimed at the next 25 years and beyond. It encompasses a broad range of technologies to meet future needs of the aviation community. Two key areas of focus are the transition to ultra-efficient subsonic transports as well as the transition to safe, quiet and affordable vertical lift air vehicles. In support of these technology areas, NASA has been researching hybrid-electric as well as fully electric aircraft designs.



Both designs necessitate the development of higher energy density battery systems. Lithium-oxygen batteries have been proposed as a potential enabling technology owing to its high theoretical energy density, to date the highest of any proposed battery technology.



However, there are immense technical challenges facing their development, including the development of more stable cathodes and electrolytes. Through a synergistic approach utilizing computational modeling and experimental screening, several new cathode and electrolyte candidates have been screened. Concurrently, decomposition analysis of candidate electrolyte systems using nuclear magnetic resonance (NMR) spectroscopy has yielded mechanistic insight into decomposition pathway, which is vital to the development of future stable electrolyte candidates.

State-of-the-art Electrolyte

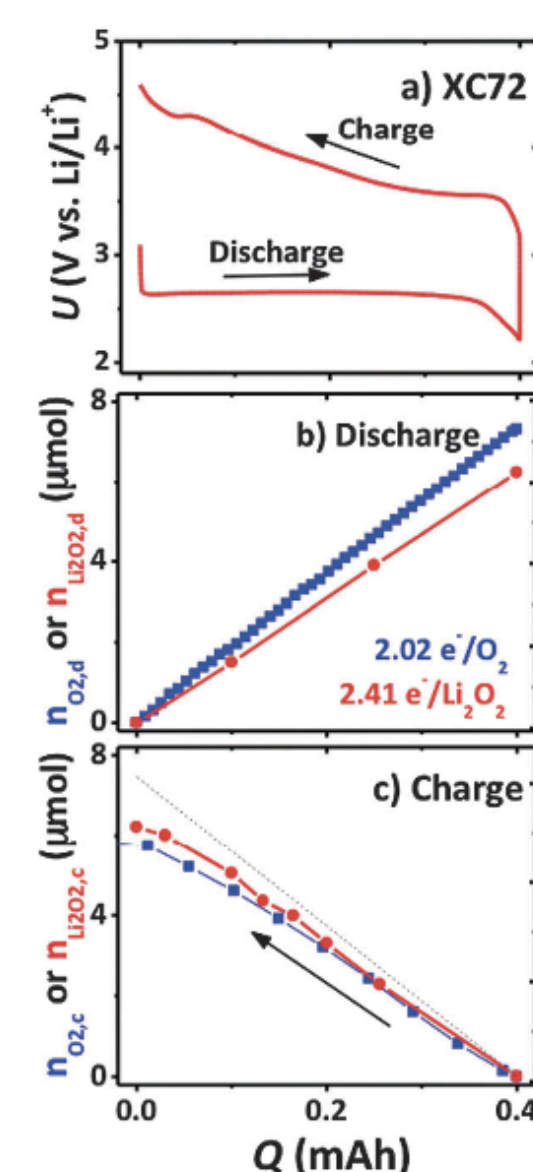
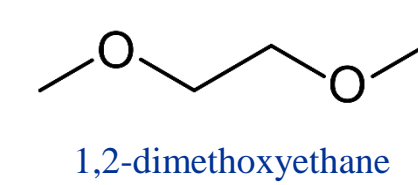


Figure 1: OER/ORR ratio of selected electrolytes and DEMS analysis of state-of-the-art electrolyte DME

Experimental

Differential electrochemical mass spectrometry (DEMS) and nuclear magnetic resonance (NMR) spectroscopy were performed on a series of amides and ureas to elucidate the decomposition mechanism of these two classes of electrolytes. Figure 2 shows the series of amides and ureas tested.

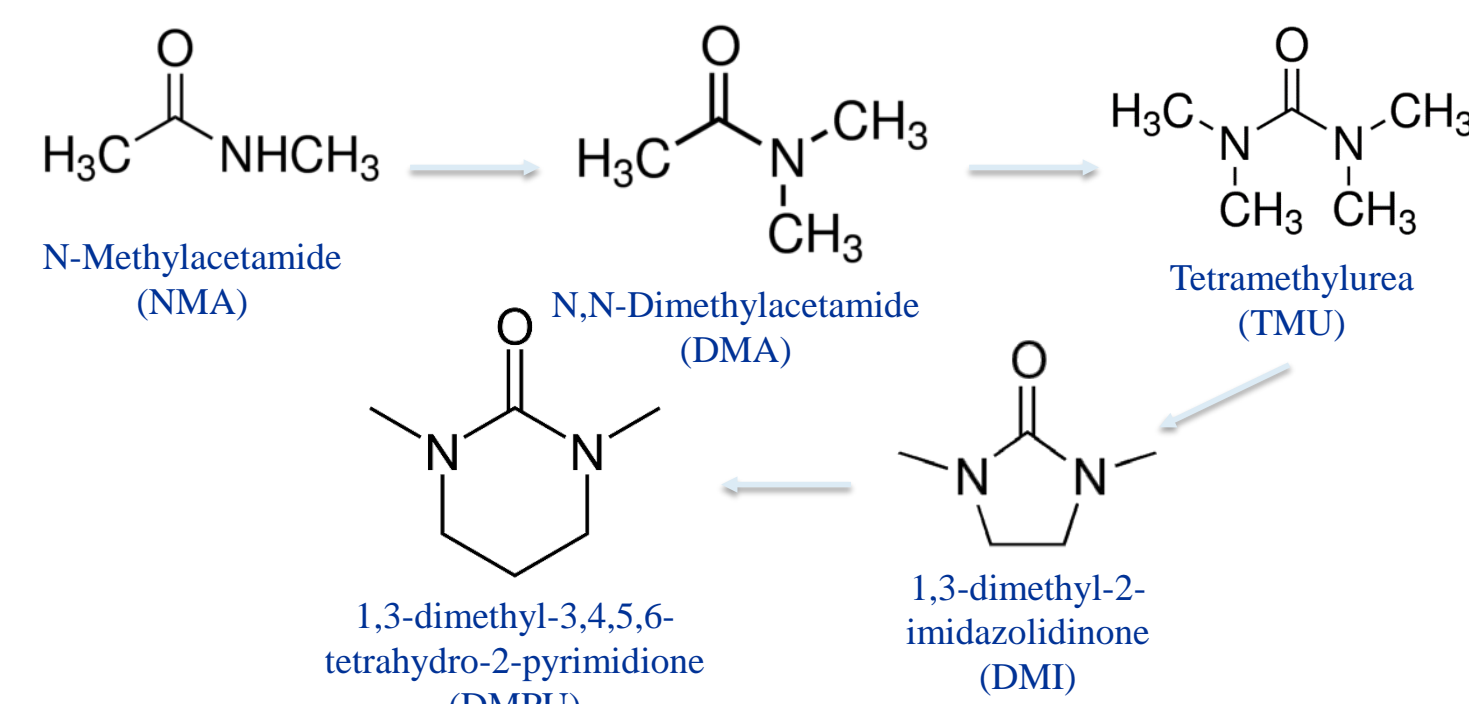
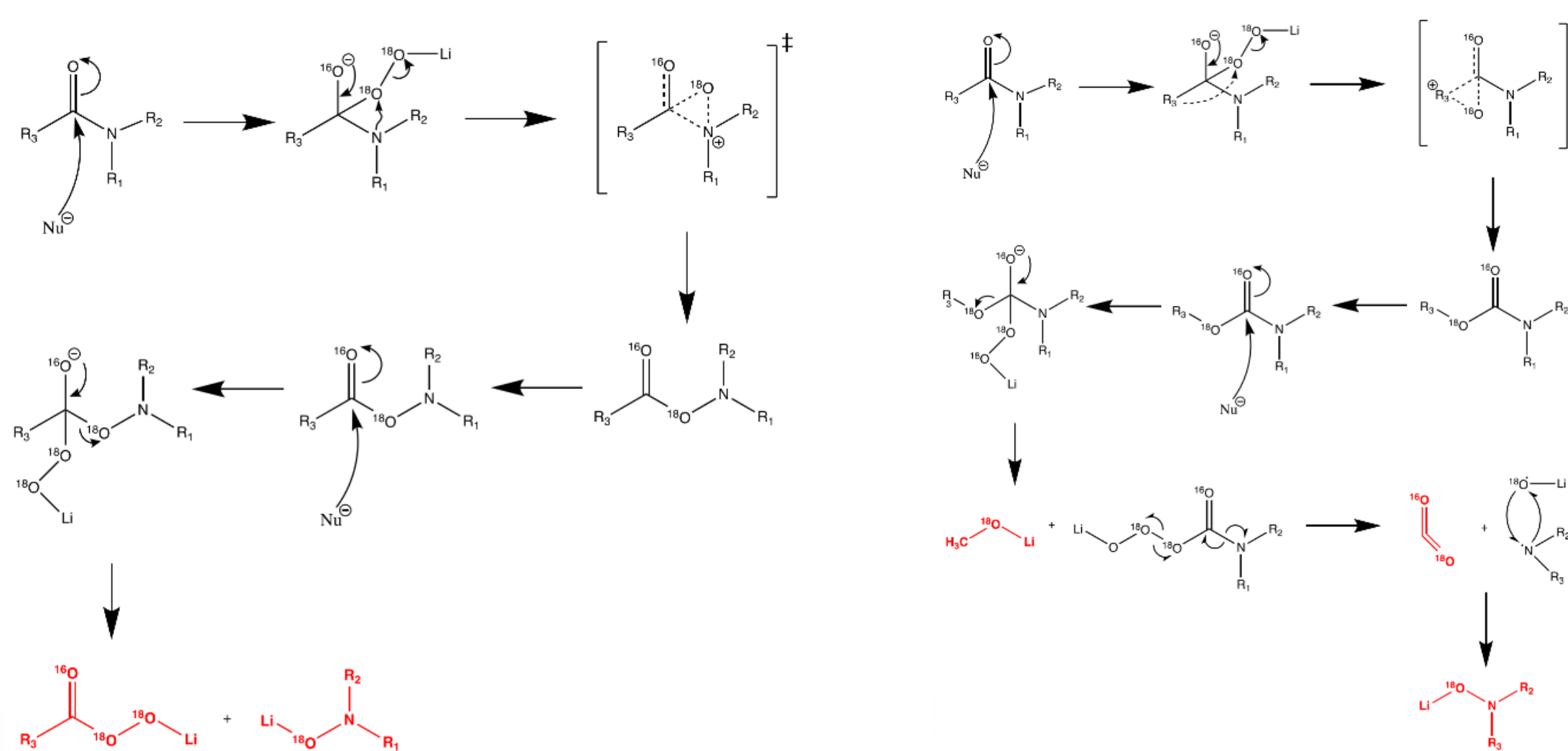


Figure 2: Series of acetamide, linear urea and cyclic urea electrolyte candidates

Results



Scheme 1: Baeyer-Villiger Oxidation of acetamide electrolytes

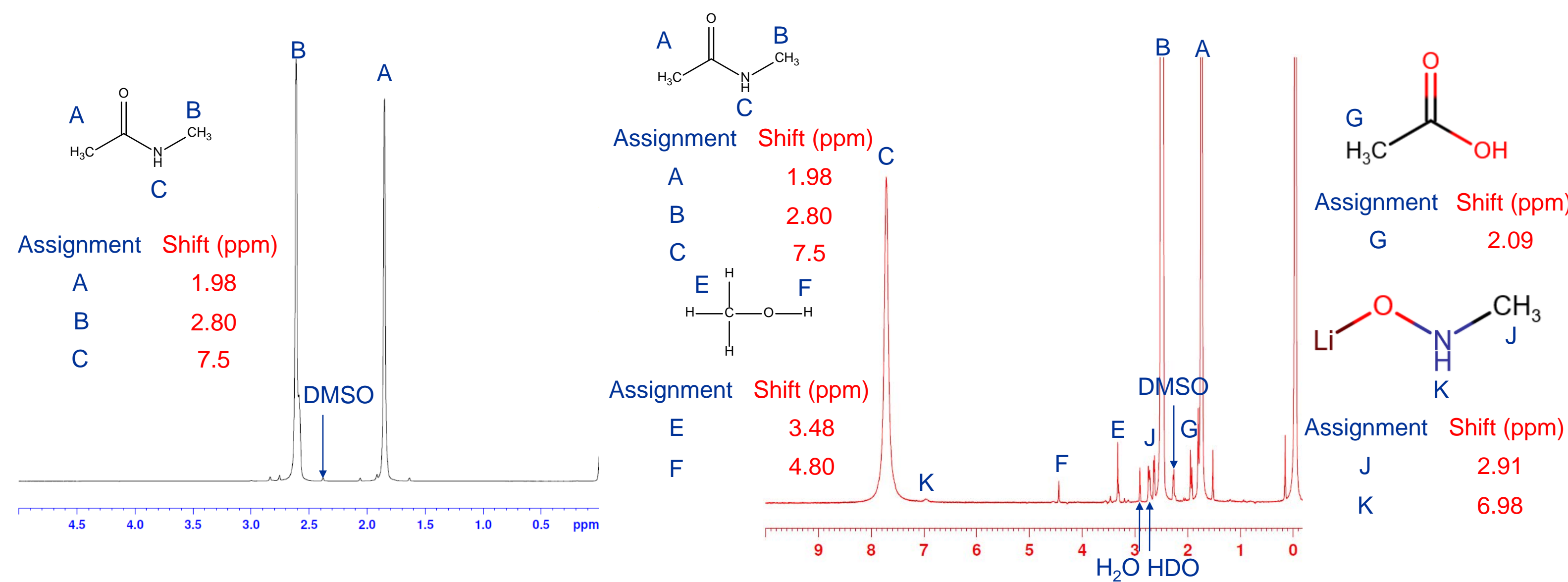


Figure 3: NMR spectra of neat NMA and the products formed after 1 cycle

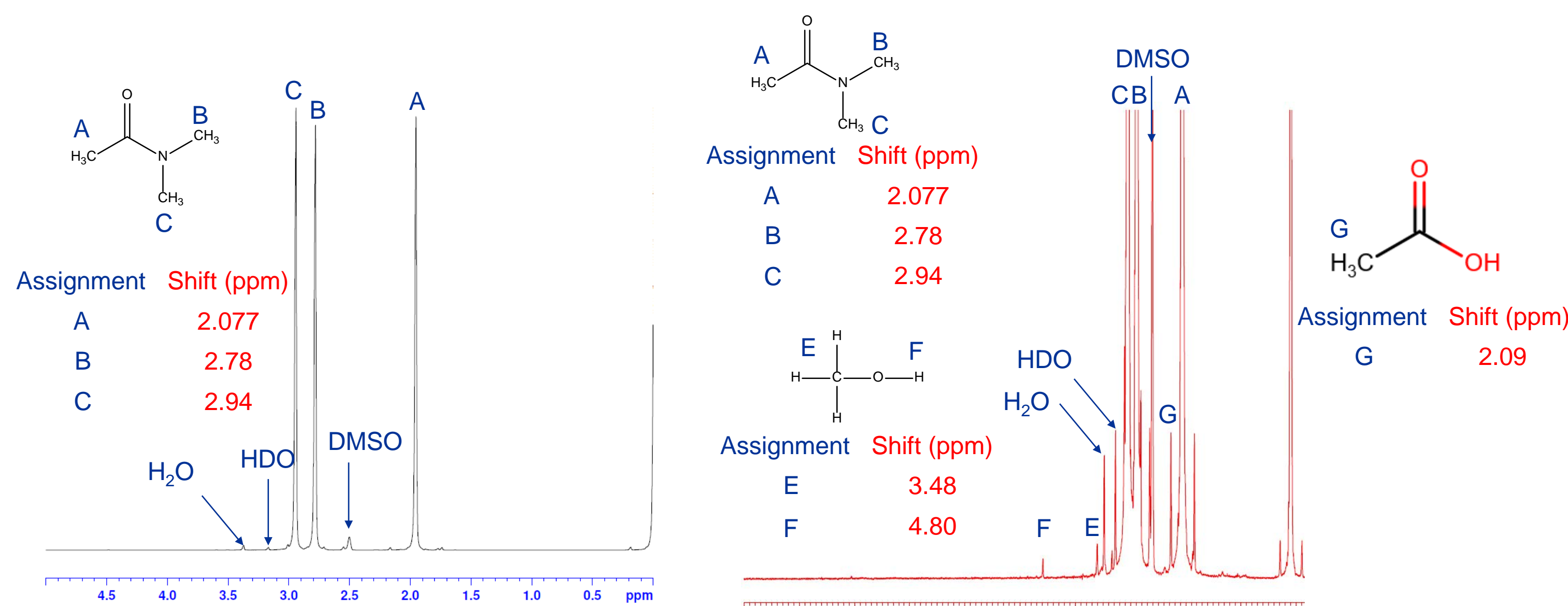


Figure 4: NMR spectra of neat DMA and the products formed after 1 cycle

Results

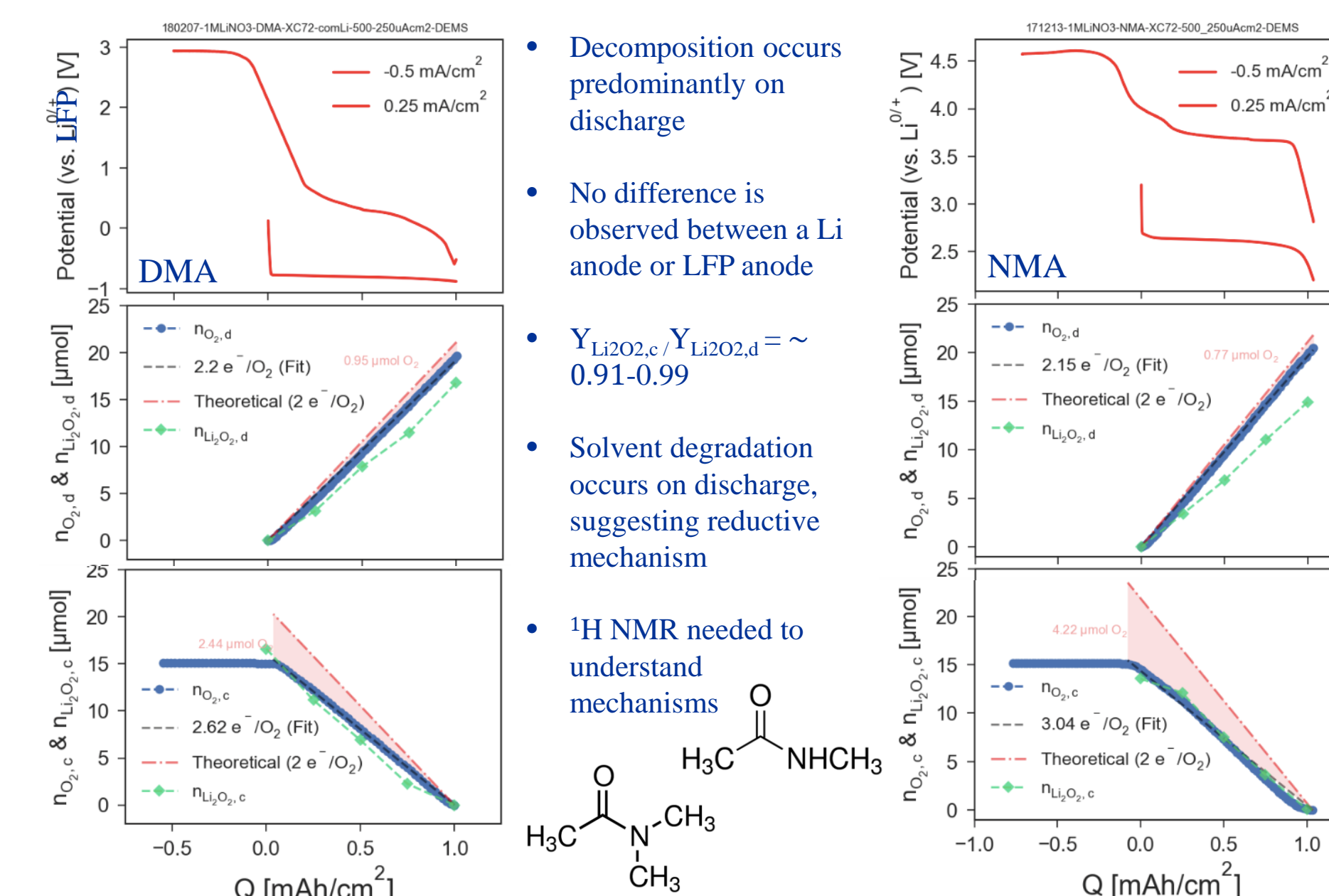


Figure 5: DEMS analysis performed for NMA and DMA in 1M LiNO₃

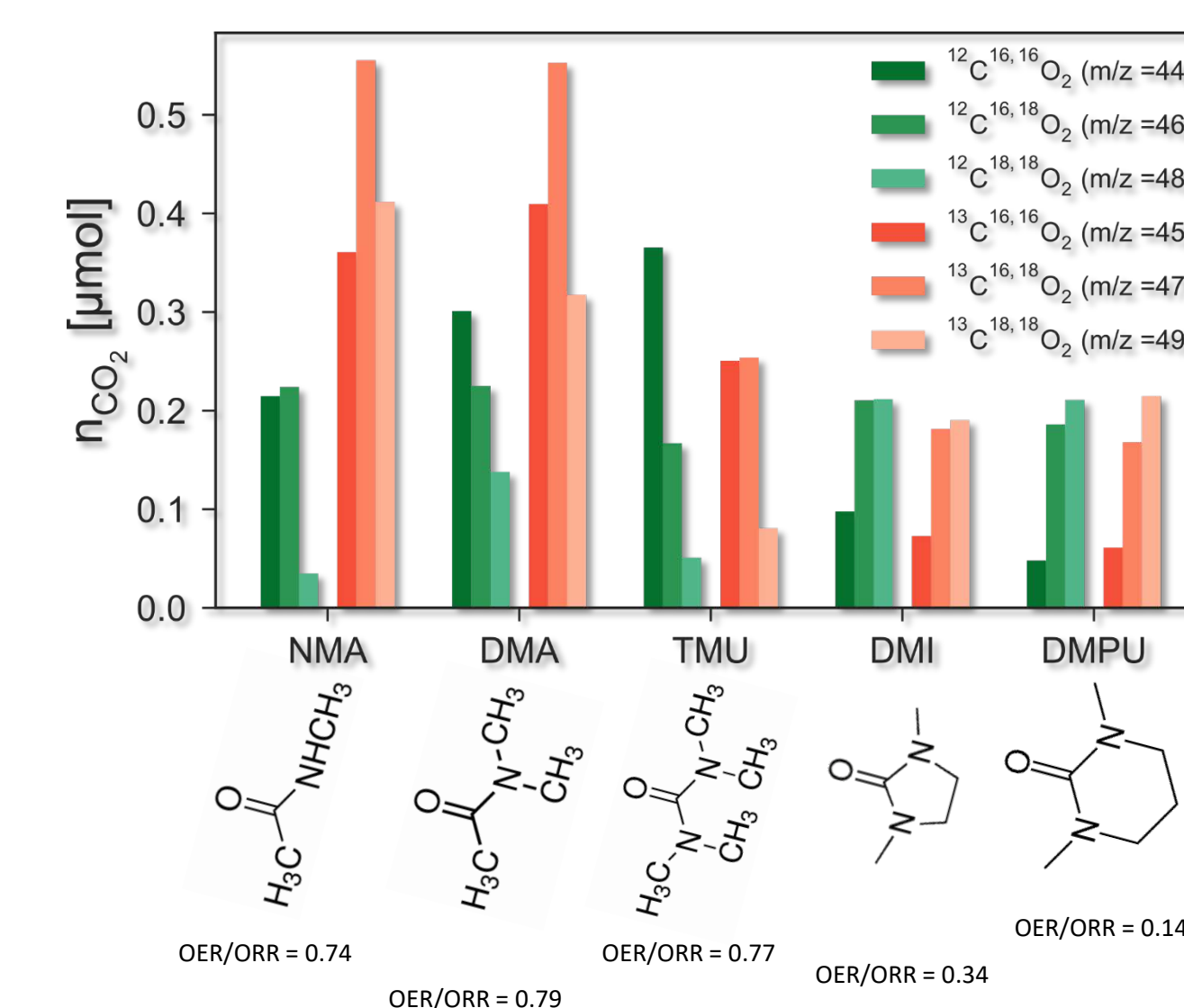


Figure 6: CO₂ evolution overview of selected amide and urea electrolytes with a focus on solvent ¹²C

Conclusions

Linear Amides (NMA, DMA)

Interestingly more ¹²C^{x,x}O is formed during charge relative to other solvents, suggesting more simple products are formed

Low amounts of ¹²C^{18,18}O₂ is formed, suggesting solvent is relatively stable towards Li₂O₂ and its intermediates

DMA shows the best stability of the amides/ureas tested, but decomposes through a Baeyer-Villiger oxidation method

Linear Urea (TMU)

Relatively low amounts of ¹²C^{18,18}O₂ formed, is more stable towards Li₂^{18,18}O₂/Li^{18,18}O₂⁻/^{18,18}O₂⁻ than linear amides

Cyclic Ureas (DMI and DMPU)

Large amounts of ¹²C^{16,18}O₂ and ¹²C^{18,18}O₂ are formed while low amounts of ¹²C^{16,16}O₂ is formed

This suggests an increased activation of a different pathway where CO₂ is formed from Li₂O₂ induced solvent reduction