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QUEEN'S UNIVERSITY
IONIC LIQUID
LABORATORIES

QUILL

Manipulating cation Lewis acidity to create functional ionic liquid systems

Aloisia King

Abbreviations

CTM - Charge Transfer Material

DihydroMAc- 10-methyl-9,10-dihydroacridine

FLP- Frustrated Lewis Pair

HIA - Hydride Ion Affinity

IL - Ionic Liquid

LA - Lewis Acid

LB - Lewis Base

[Lut-H][NTf_2] – [Lutidinium-H][NTf_2]

[NTf_2] - Bistriflimide

1,3,5-TMB – 1,3,5-Trimethoxybenzene

Overview

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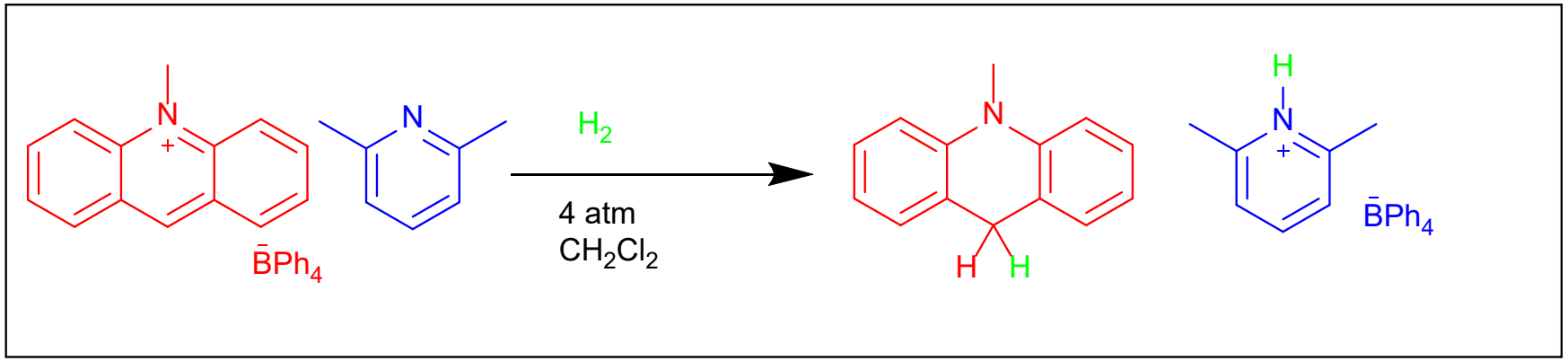
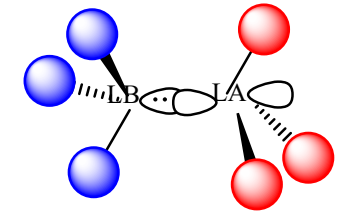
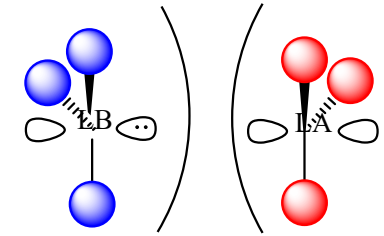


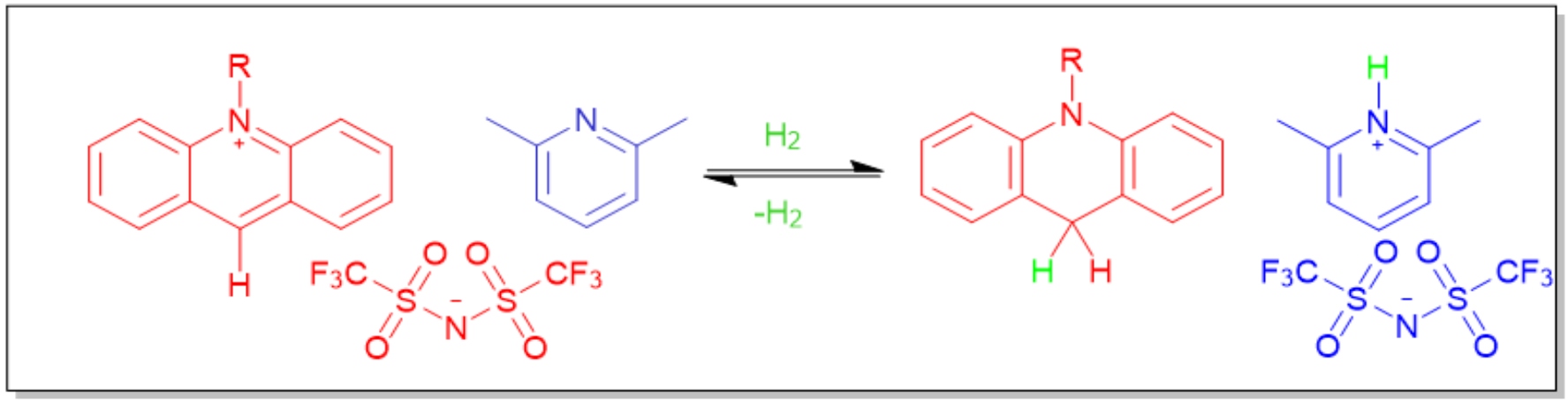
E. R. Clark and M. J. Ingleson, *Angew. Chem., Int. Ed.*, 2014, 53, 11306–11309.

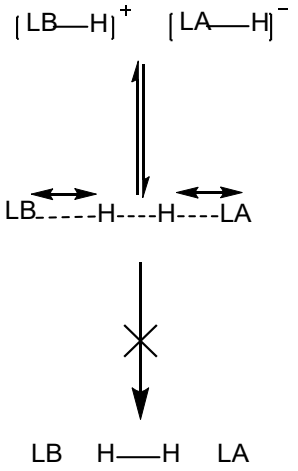


Classical Lewis adduct



Frustrated Lewis Pair





Ability to utilize range of New LA cations

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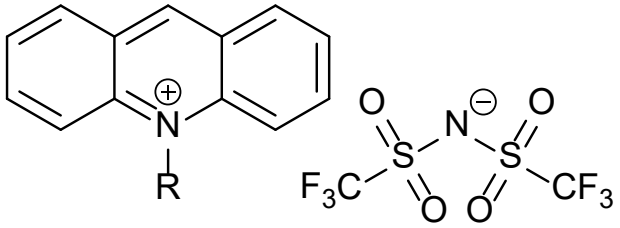
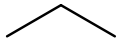
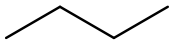
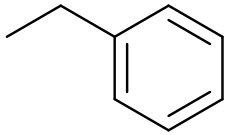
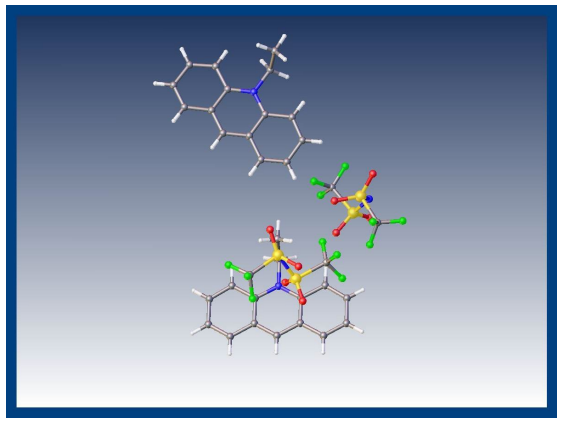
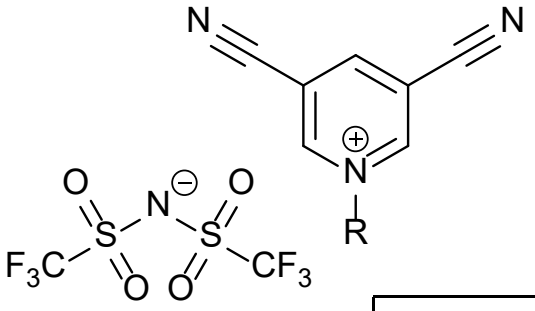


R Group







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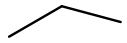
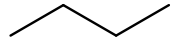
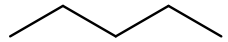
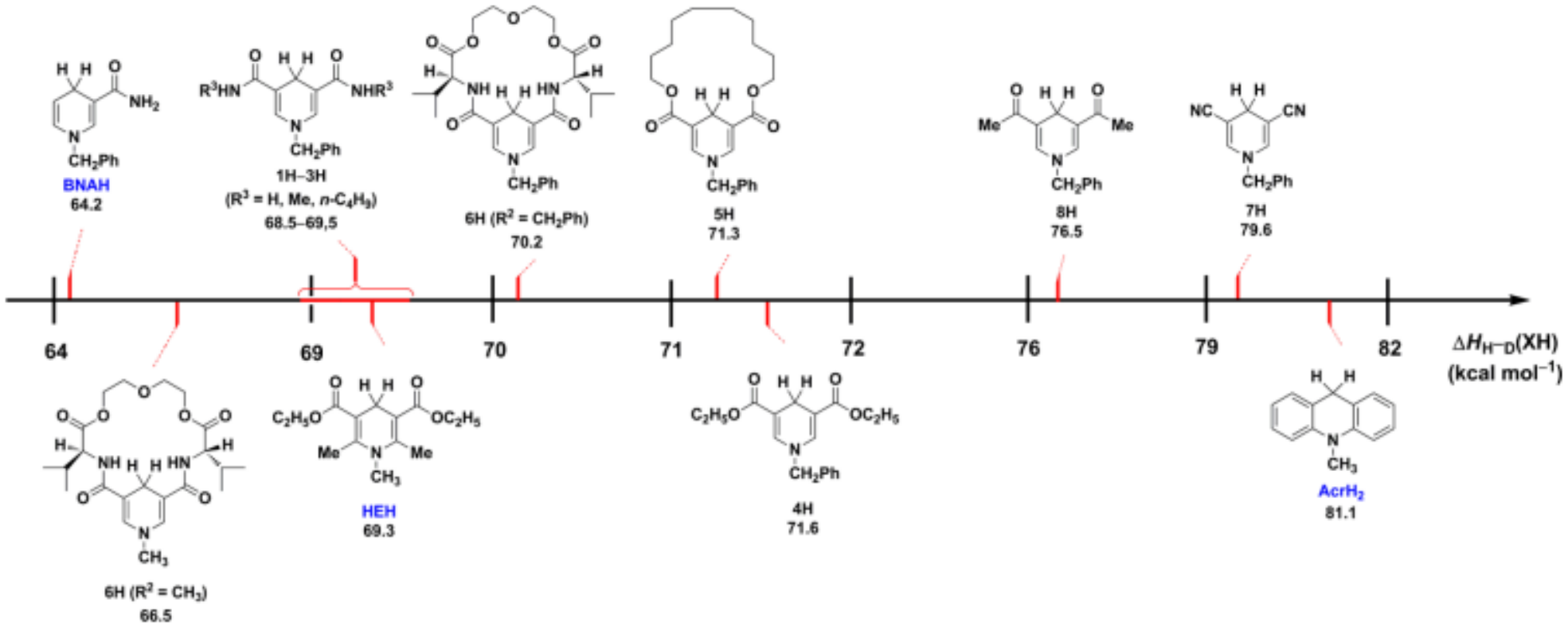




Inspired by HIA



(copied from , H. Zhao, L. Yang and X.Q. Zhu. *ACS Omega* 2018, 3, 13598−13608

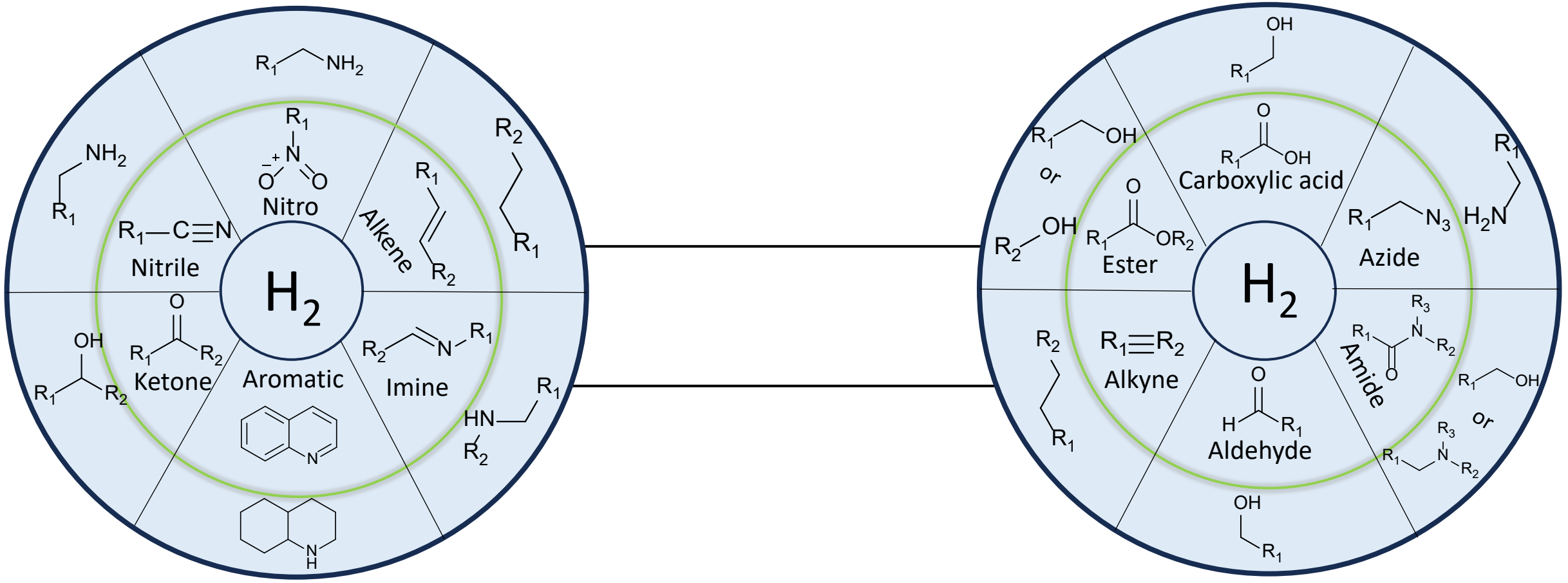
The HIA measures the **stability** of a carbocation (a positively charged carbon atom) by assessing how readily it can accept a hydride ion (H^-)

A higher HIA indicates greater stability for the carbocation

D.J. Goebbert, P.G. Wenthold. *International Journal of Mass Spectrometry,* 257 (2006) 1–11

Uses of catalysts…

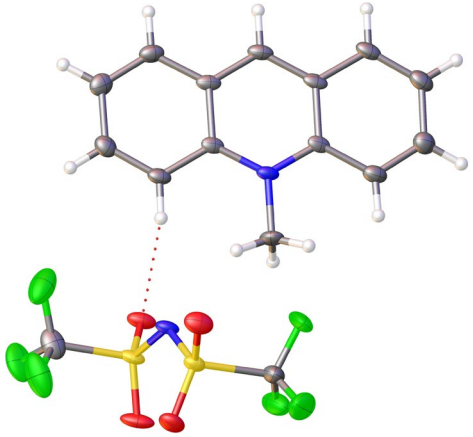
Petrochemical, Pharmaceutical, Agrochemical, Environmental, Food & Coal Industries

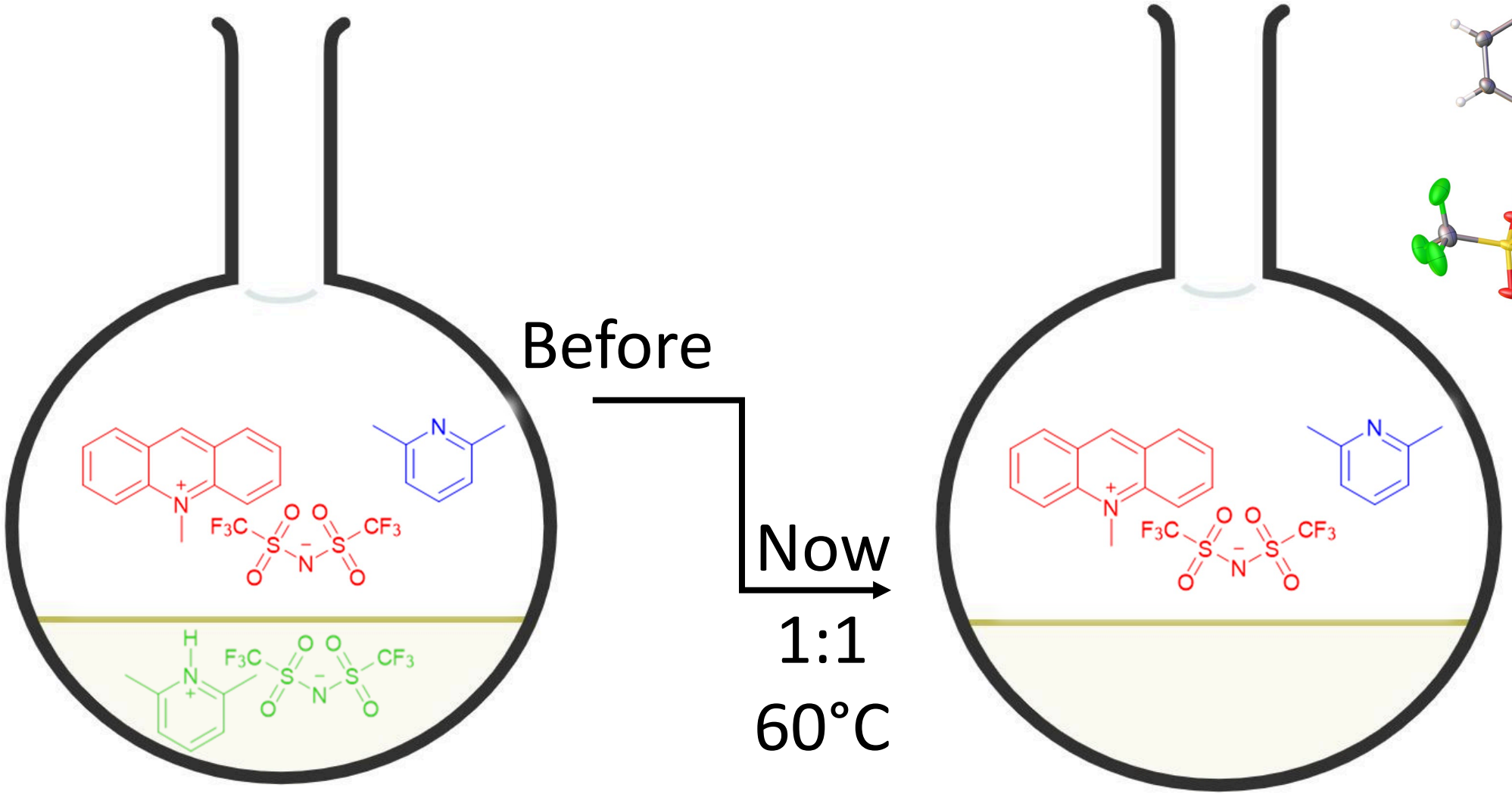


Development of intrinsically IL FLP system

100 % H_2 gas

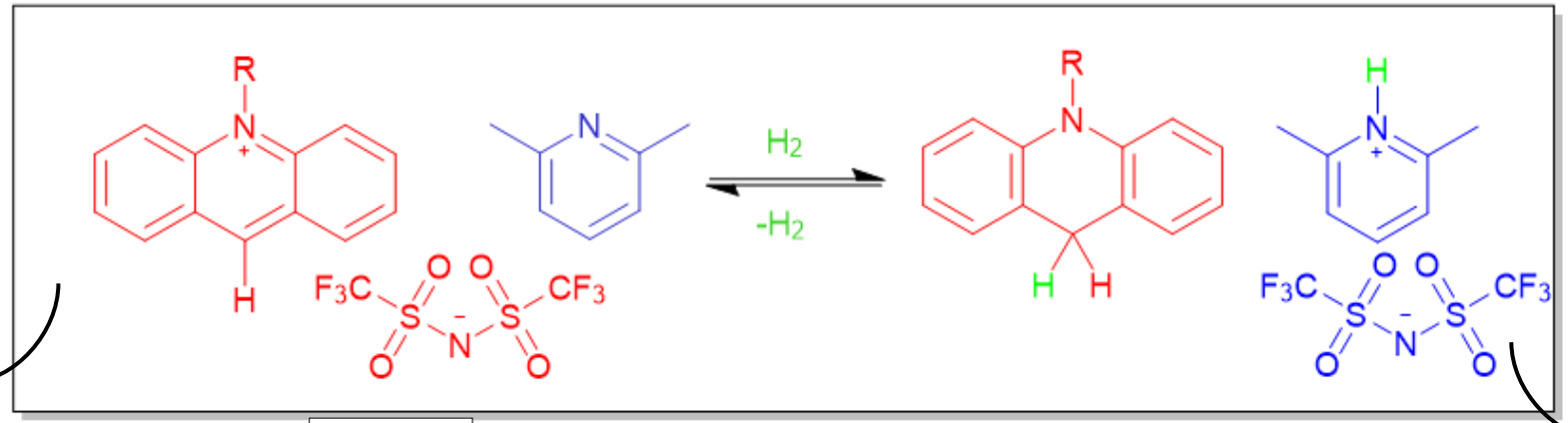
5 % H_2 gas in N_2

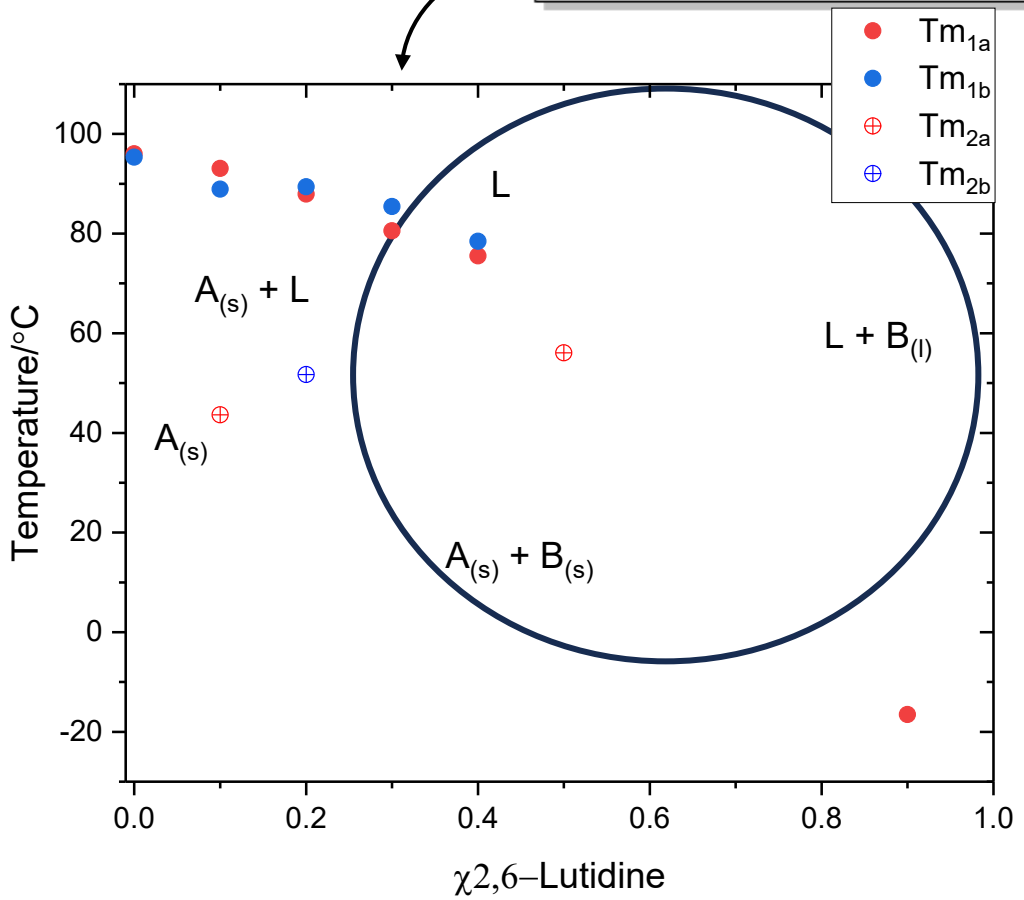


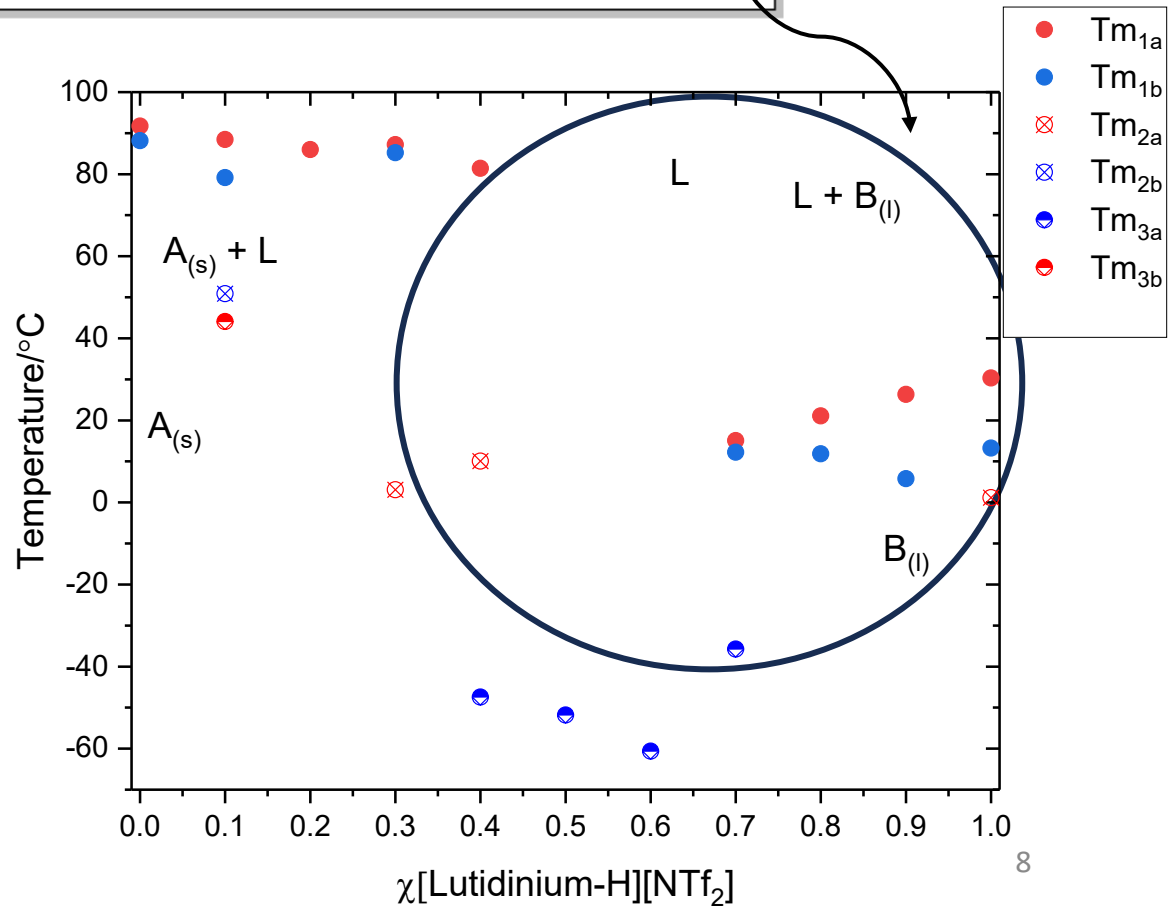


2.1 x 10^{-3} moles of FLP and 5 x 10^{-5} moles of H_2 & 20 FLPs for every H_2 in this mix

Thermal analysis







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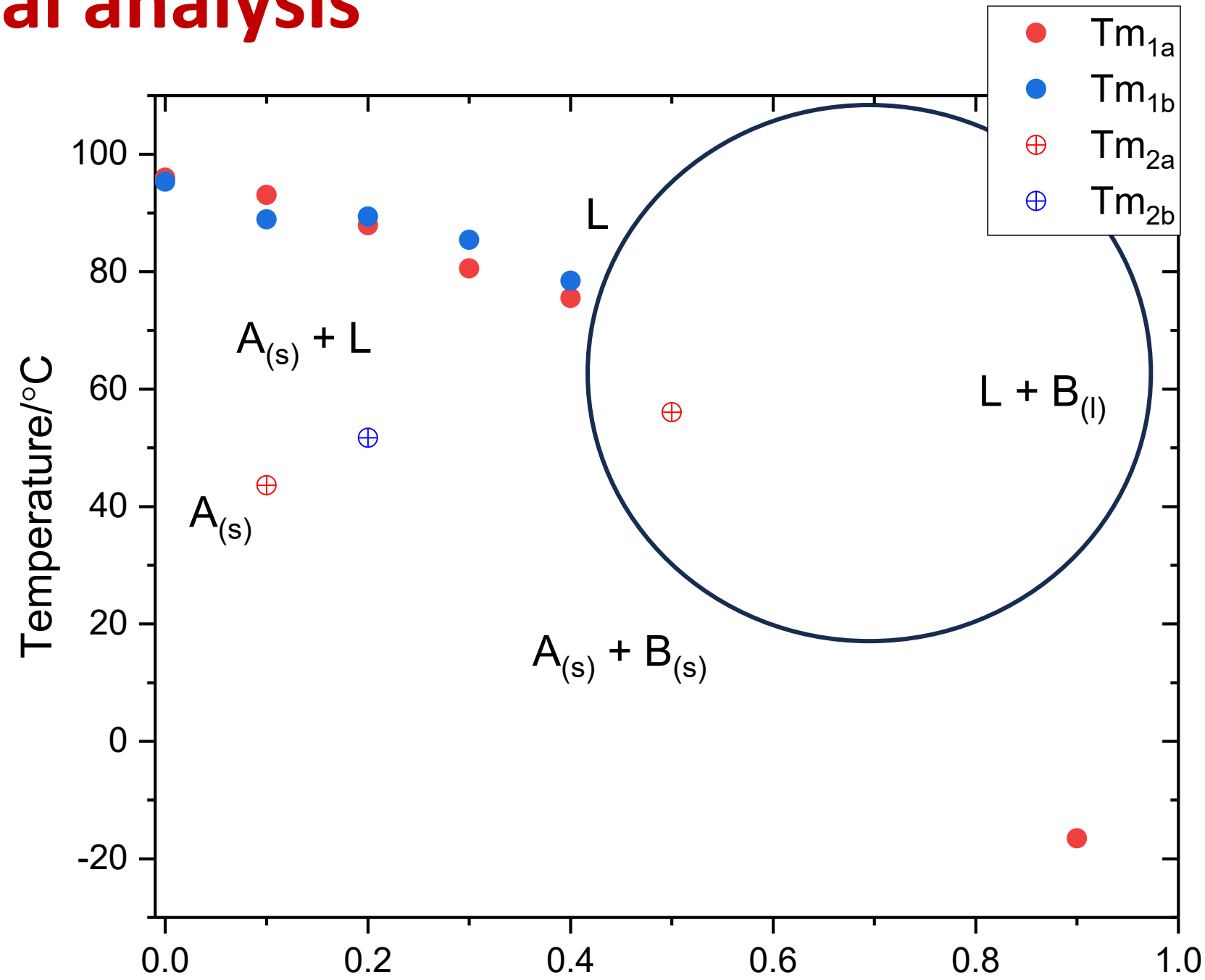

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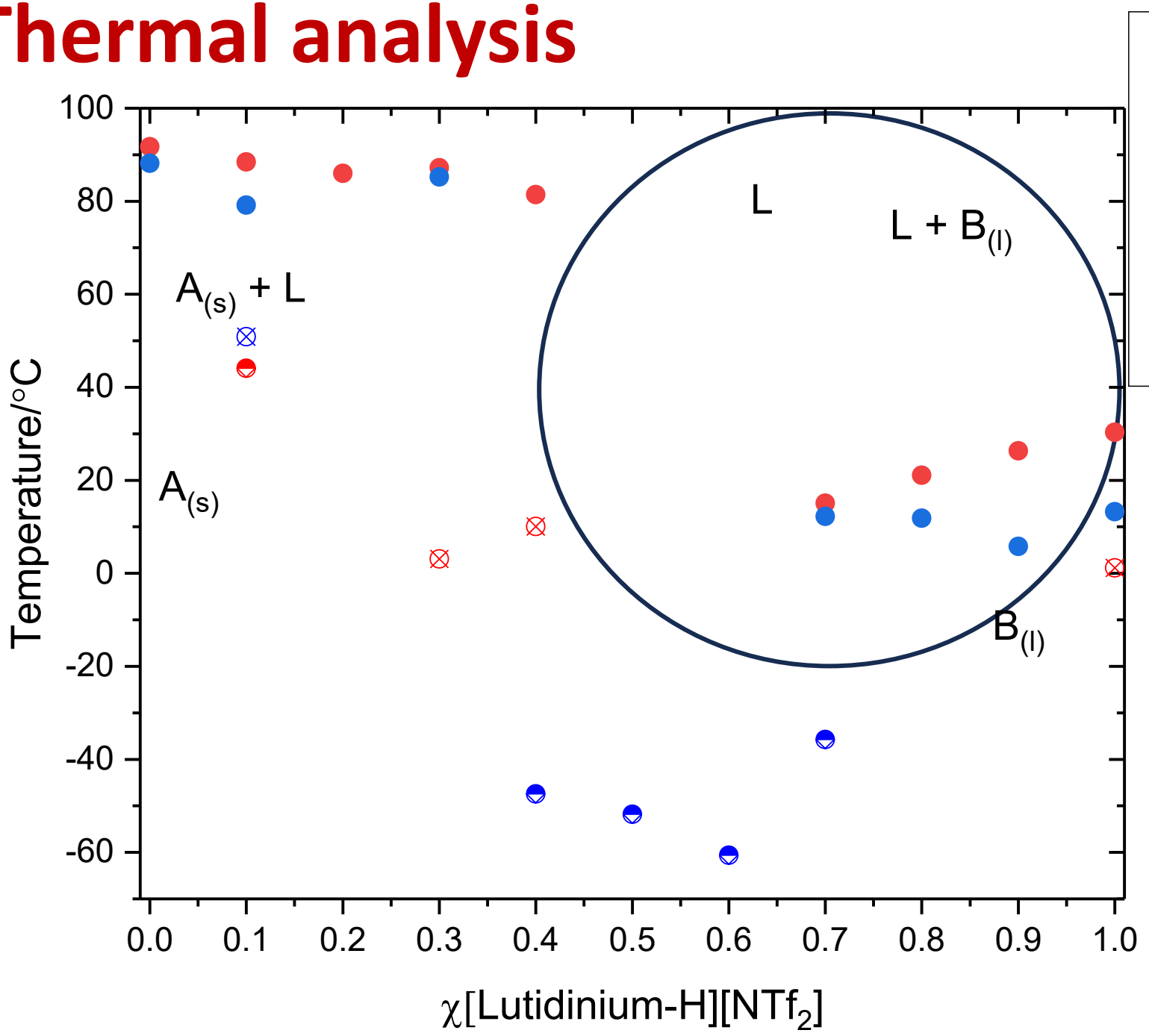
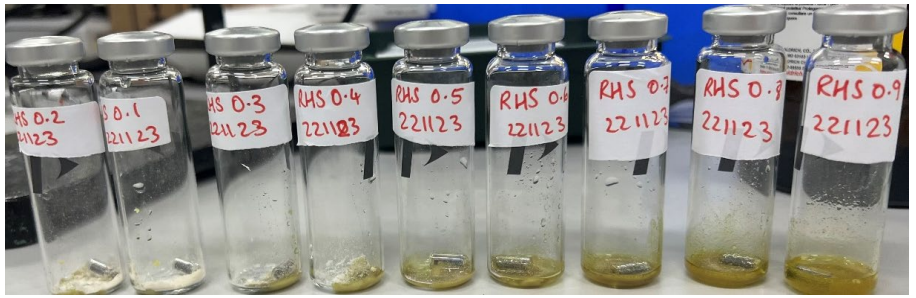
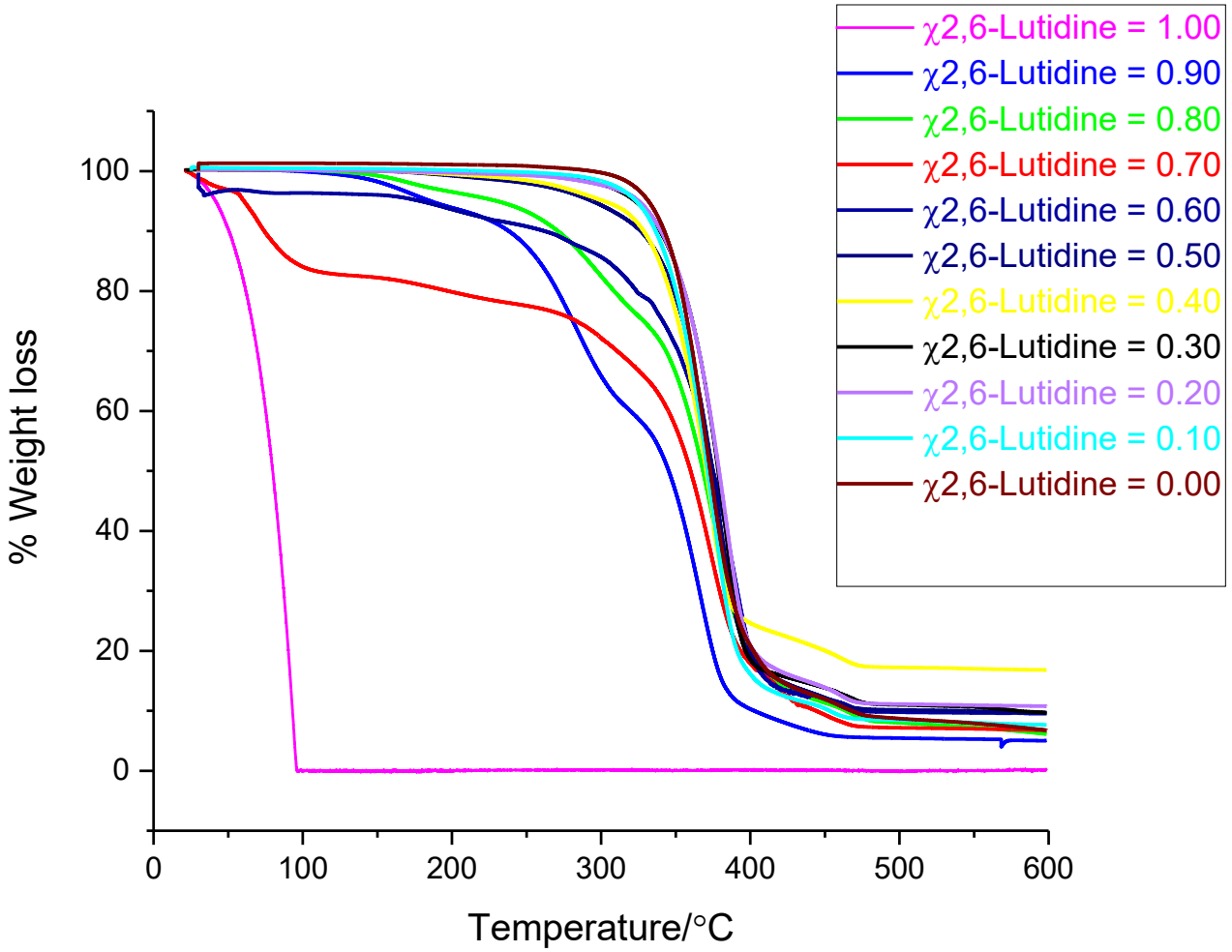
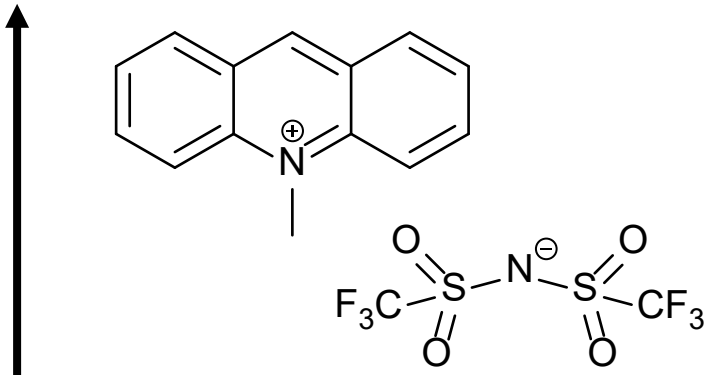


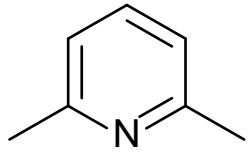


“Entrainment” of LB by LA



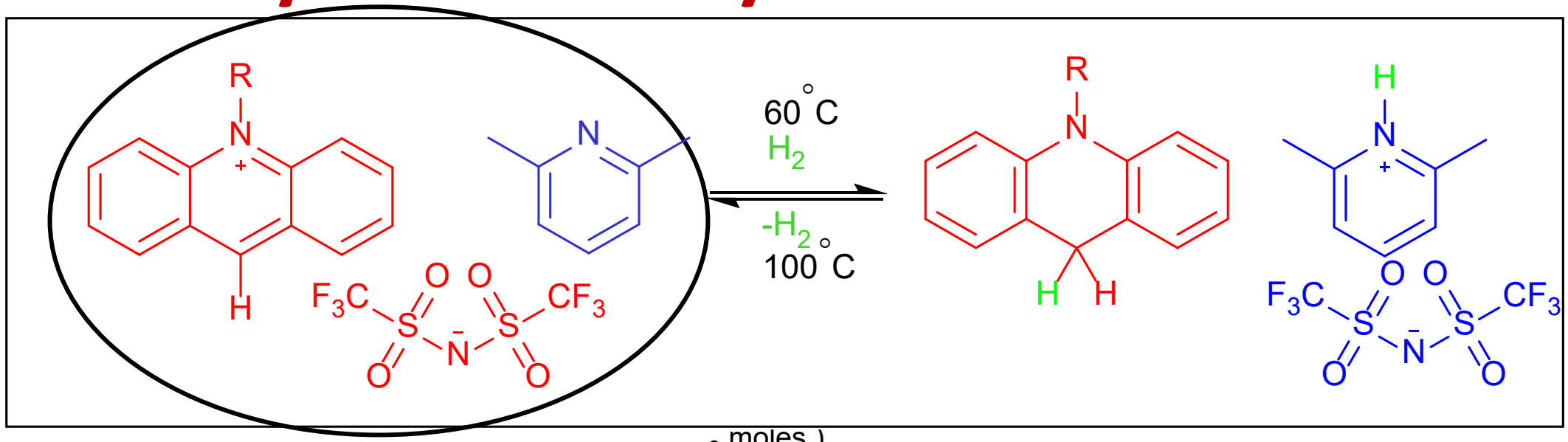


Increasing conc. of LA



Decrease in % weight loss of 2,6-Lutidine

Intrinsically IL FLP Catalysis



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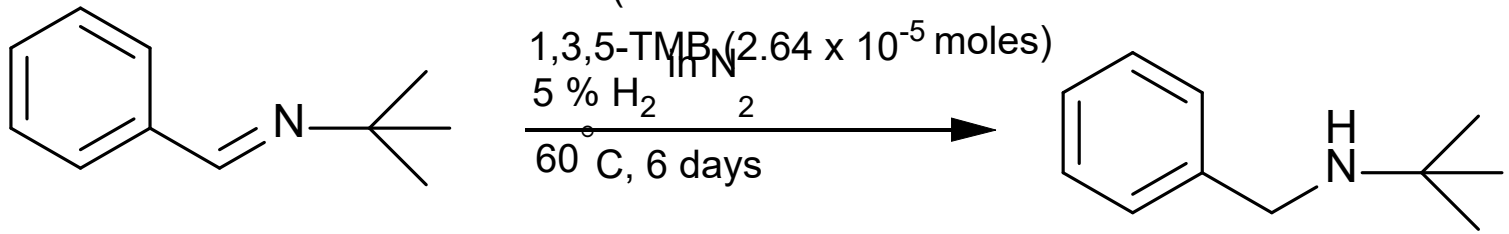

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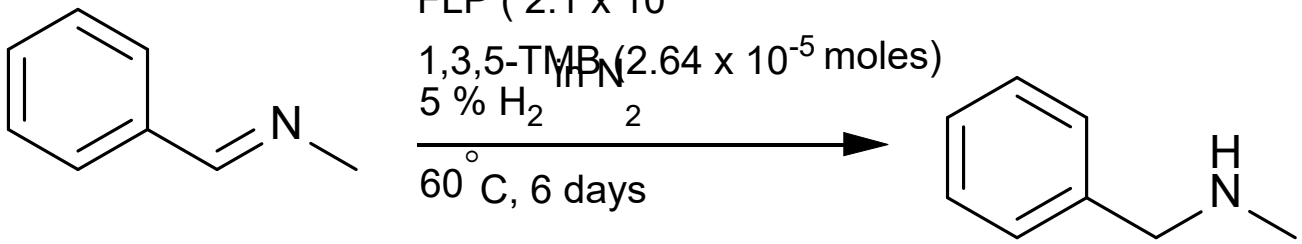

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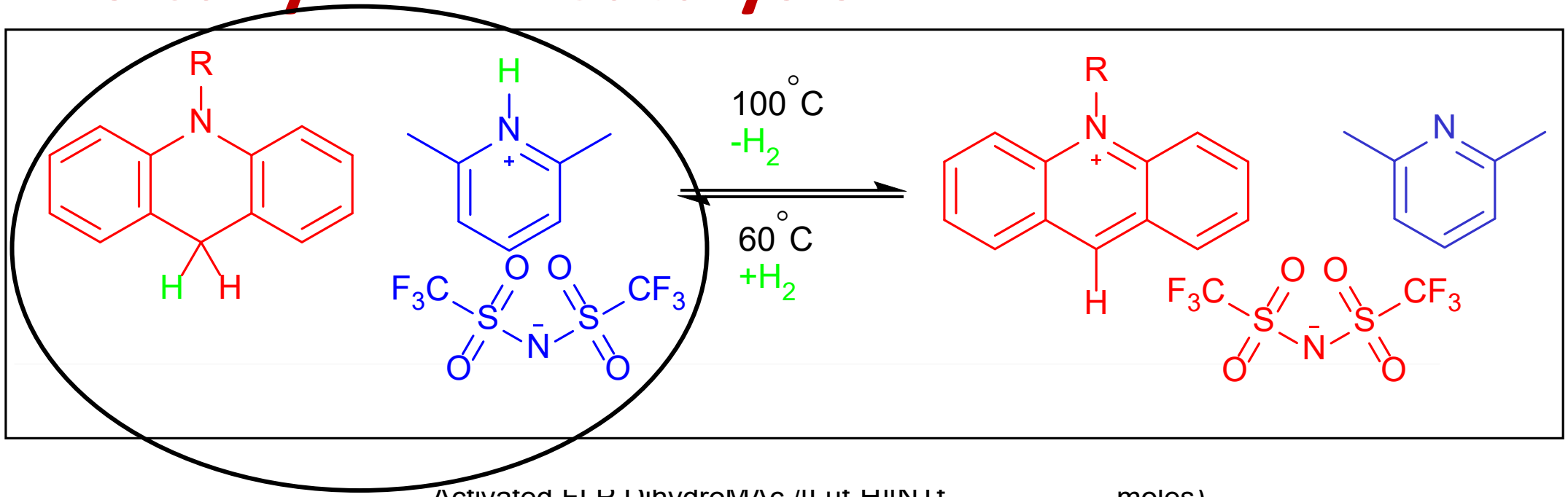
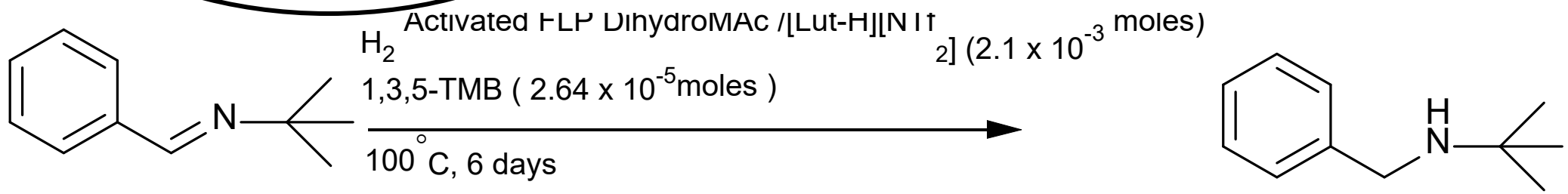
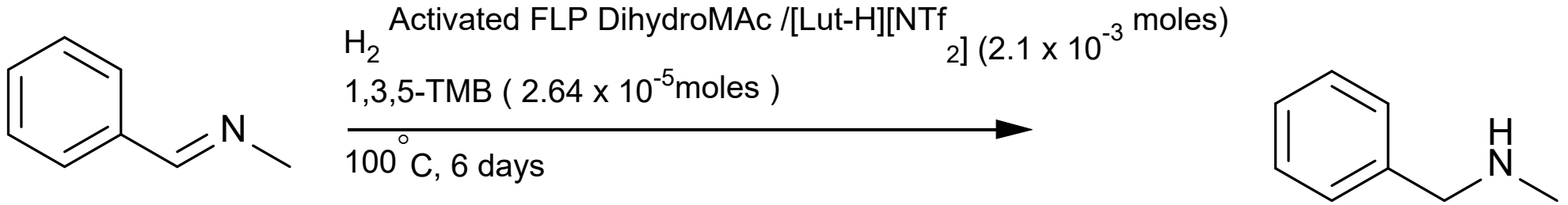
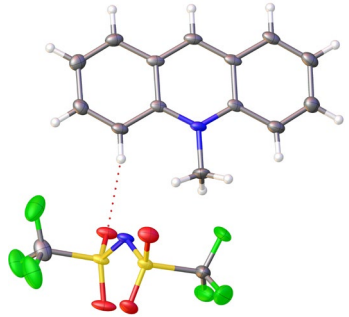






Future work & Conclusions



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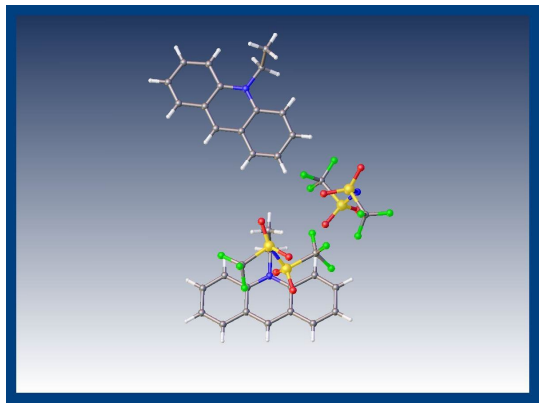
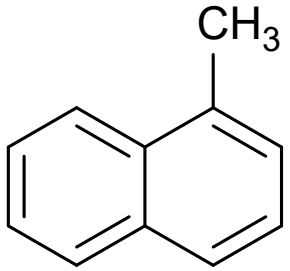
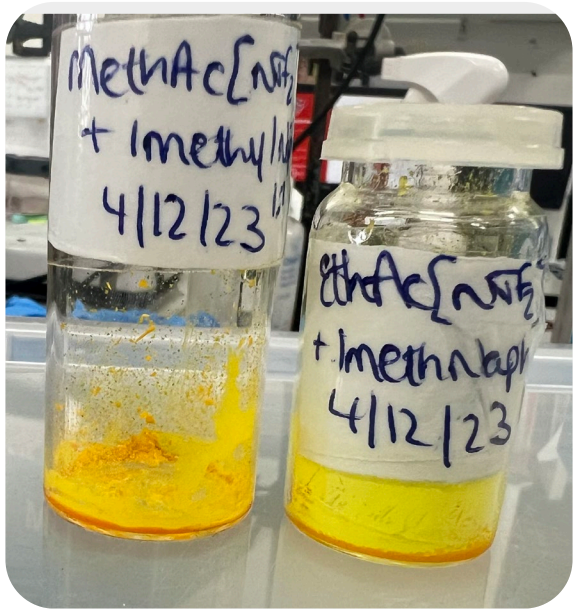
- Deuterate samples and take them to ISIS to probe liquid nature
- Fluorescent measurements of Individual FLP components, hydrogenated species & de-hydrogenated species
- Probe H_2 uptake in range of 3,5-Dicyanopyridinium (similar HIA) IL FLPs & Investigate these materials as CTMs
- Continue EIS of Cyanopyridinium ILs & 3,5-Dicyanopyridinium ILs – collaboration with Dr. Josh Bailey
- Test CTM behaviour of N-alkylated acridinium [NTf_2] species







Acknowledgements

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- Dr. Pete Goodrich,Miss Sanskrita Madhukaiya, Mr. Mark Young and Dr. Leila Moura

- Everyone in QUILL