QUEEN'S UNIVERSITY BELFAST

QUEEN'S UNIVERSITY IONIC LIQUID LABORATORIES QUILL

A Study of Lewis Acidity in Boron

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1. Background

Problem

Quantifying Lewis acidity is difficult as it not only depends on the identity of the acid but also on the identity of the base.

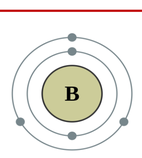
Current methods rely on NMR spectroscopic probes (Gutmann or Childs methods) or computational measurements of probe-acid interactions, (fluoride and hydride affinity scales – FIA and HIA).

Solution

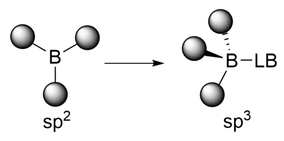
Use X-Ray spectroscopy to measure the energy of the 1s→LUMO transitions to isolate a component of Lewis acidity in a probe-free method.

Factors that affect Lewis acidity:

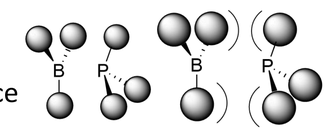
Electrotonic structure of boron centre



Energy required to change geometry

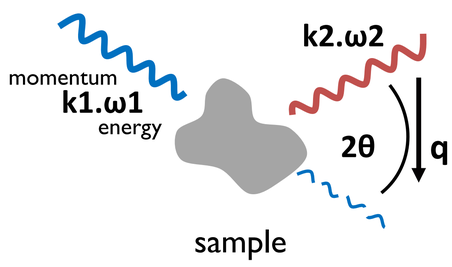


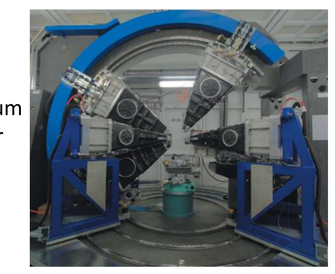
Steric hindrance



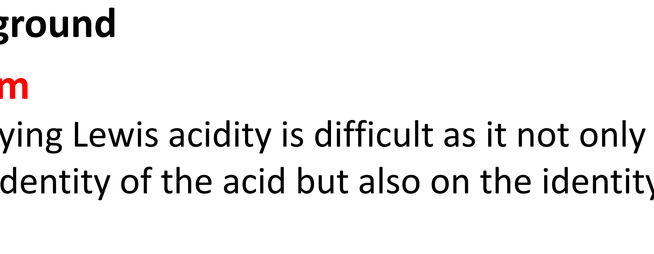
2. X-Ray Raman Spectroscopy (XRS)

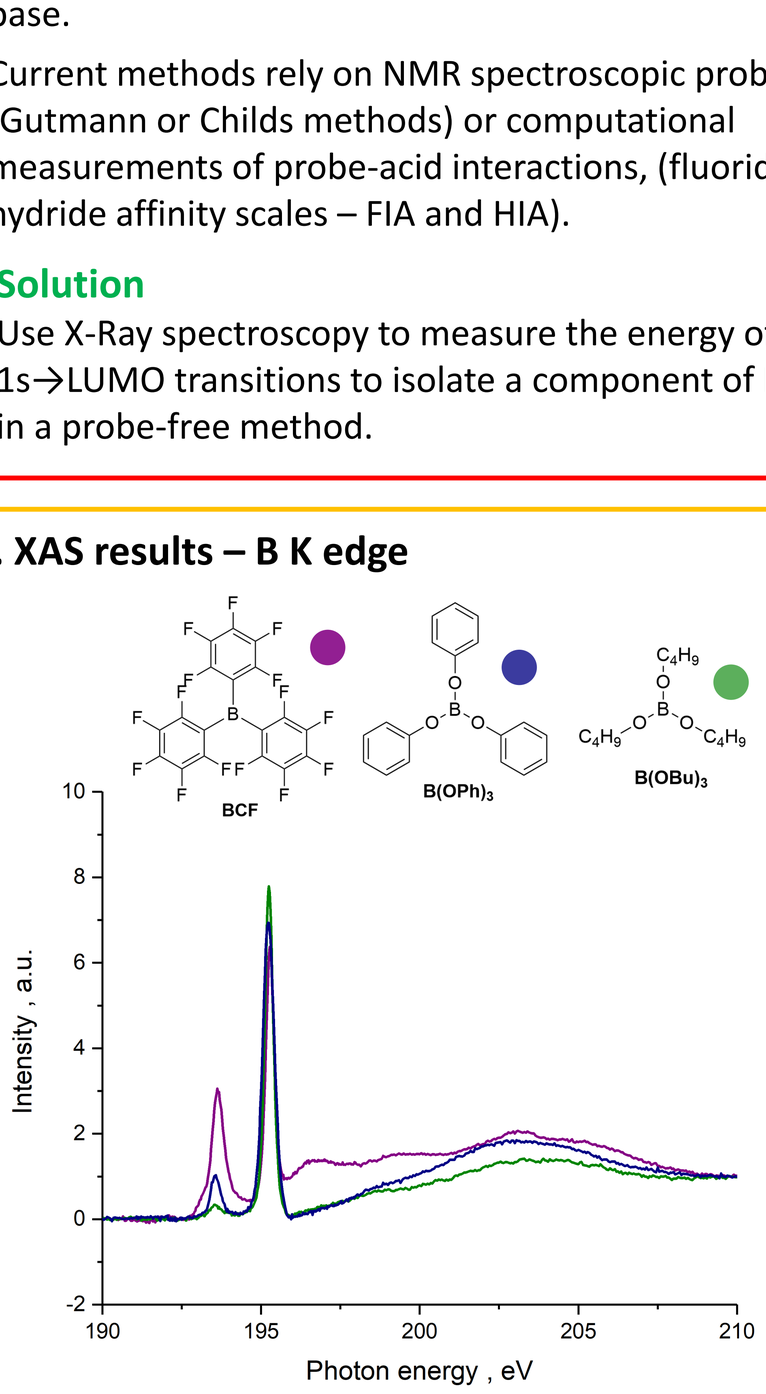
- XRS is a hard X-ray, bulk-sensitive technique that can provide equivalent information to soft XAS.
- It is the non-resonant inelastic X-ray scattering (IXS) from core-shell excitations and can be used to study the K-edge of light elements.
- this technique eliminates the need of a vacuum and allows for more complex sample environments

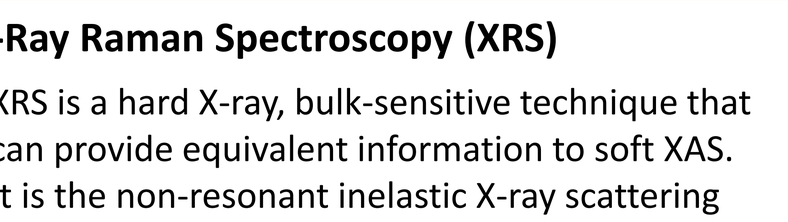




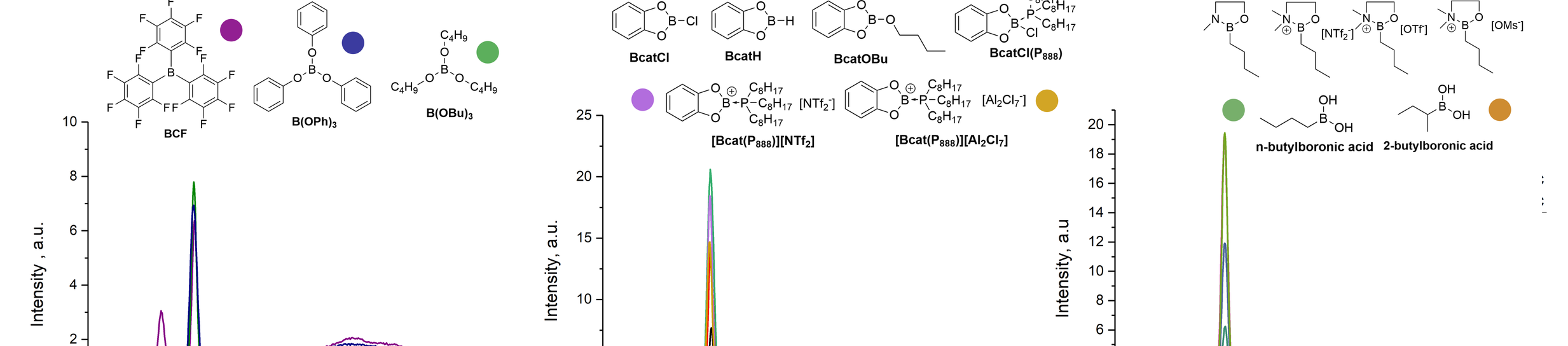
3. XAS results – B K edge







4. XAS vs XRS results – B K edge

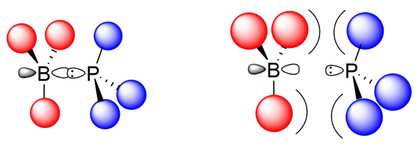


5. Conclusions

- We have measured the B K edge of a range of boron Lewis acids using XAS and XRS to measure the 1s→LUMO transition to isolate a component of Lewis acidity.

6. Future work

- We hope to continue this work to develop a new Lewis acidity scale.
- Additionally, combine these boron Lewis acids with a base in a Frustrated Lewis pair (FLP).
- Eventually conduct operando studies on hydrogenation reactions with FLP-SILP systems.



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