

Alkali Cation Size-Specific Guest Trapping in Supramolecular Complexes Characterized Using CRAFTI Collision Cross Sections



Tina H. M. Farzan*, Mariah Pay, Spencer Johnson, David V. Dearden

Tina.heravi@chem.byu.edu

Introduction

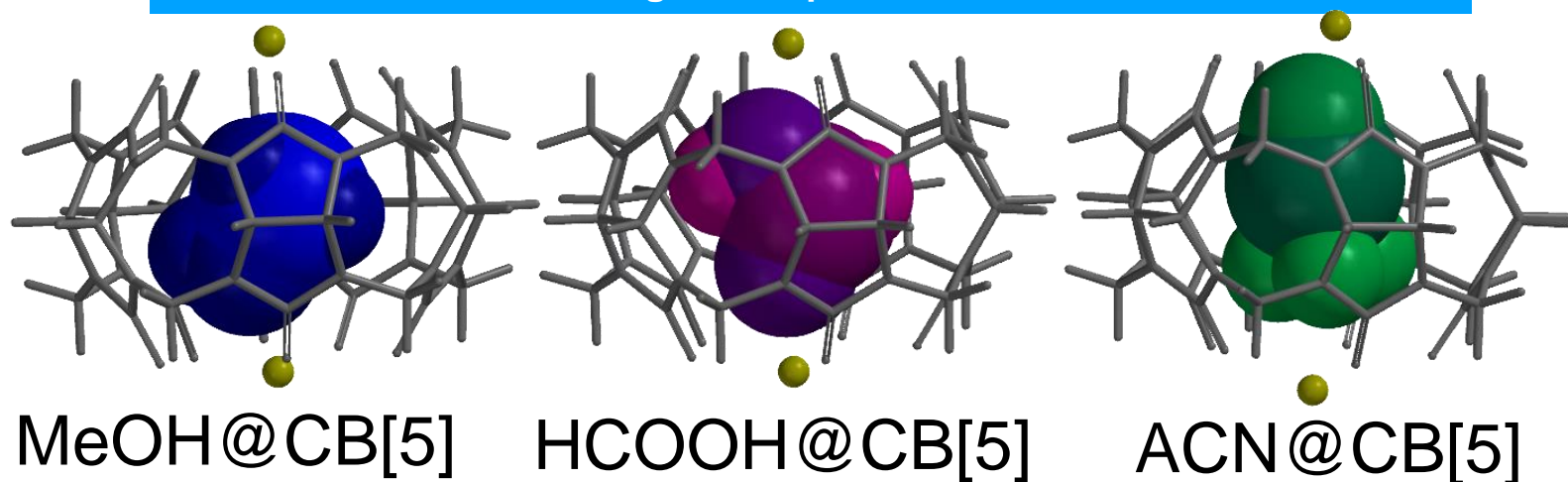
- Fourier transform ion cyclotron resonance mass spectrometer (FTICR-MS) gives accurate mass and ultra-high mass resolution
- New "CRAFTI" technique is used for measuring collision cross sections (CCS), consistent with computationally values
- "CRAFTI" = cross sectional areas by Fourier transform ion cyclotron resonance
- This study shows metal-dependent guest selectivity of Cucurbit[5]uril complexes

Methods

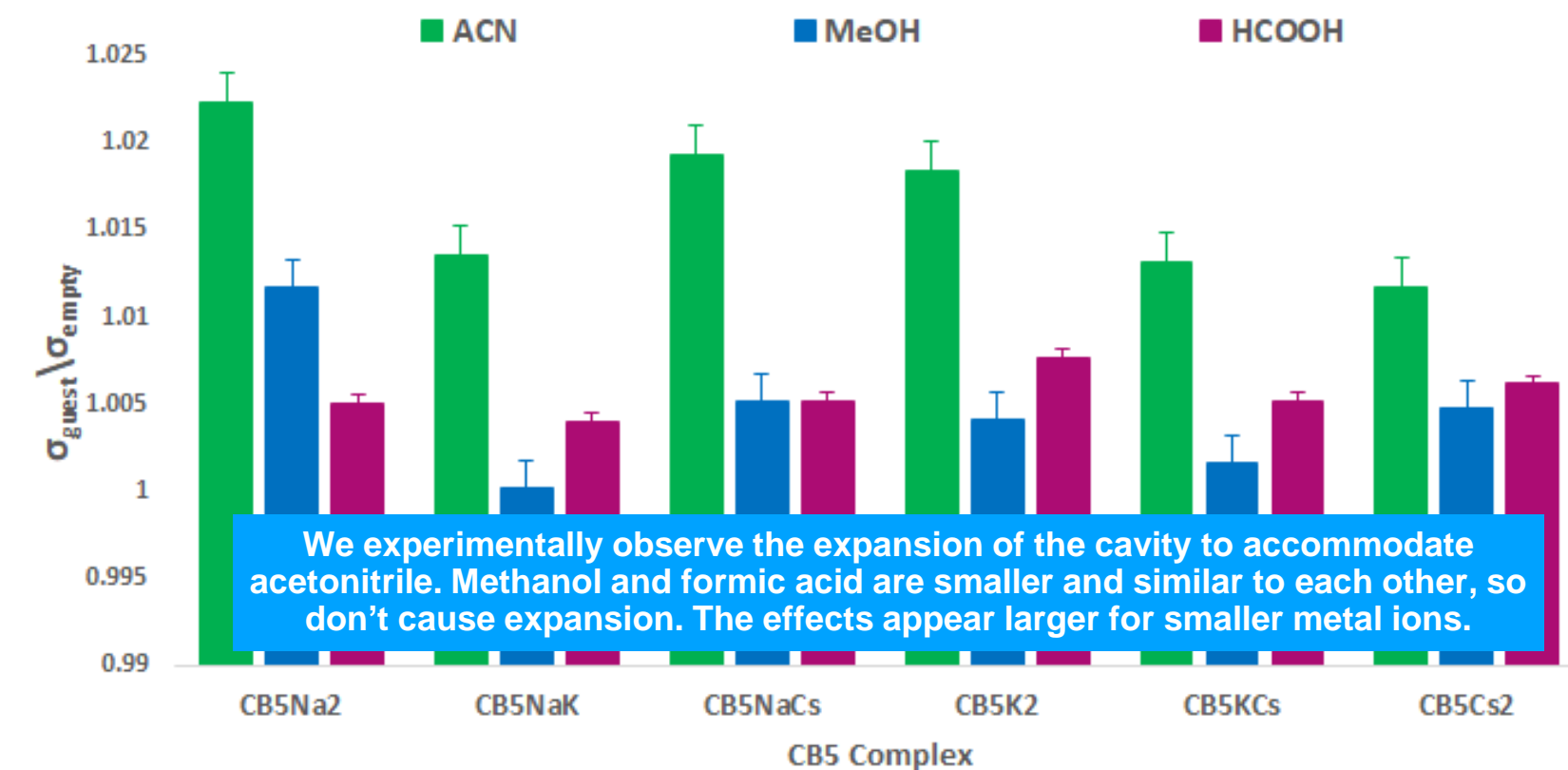
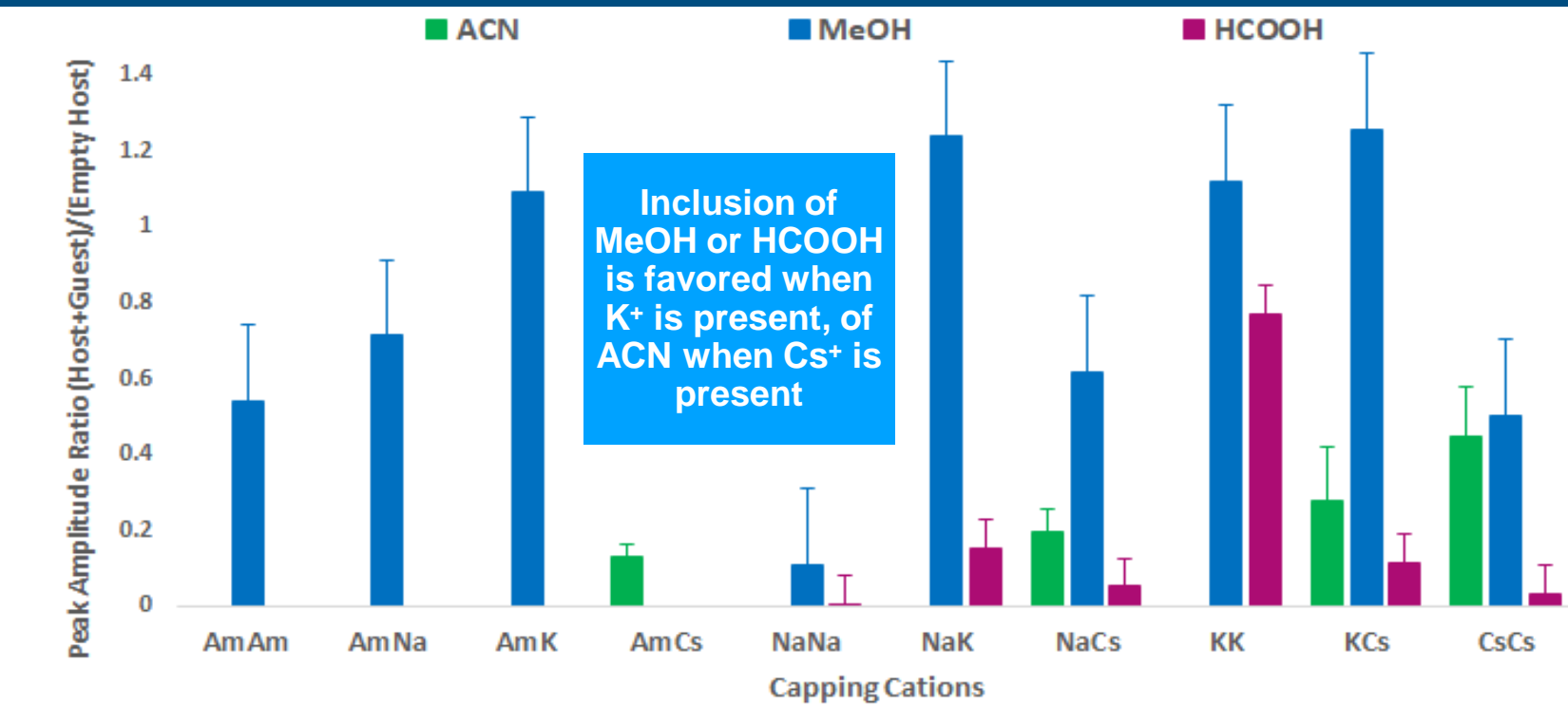
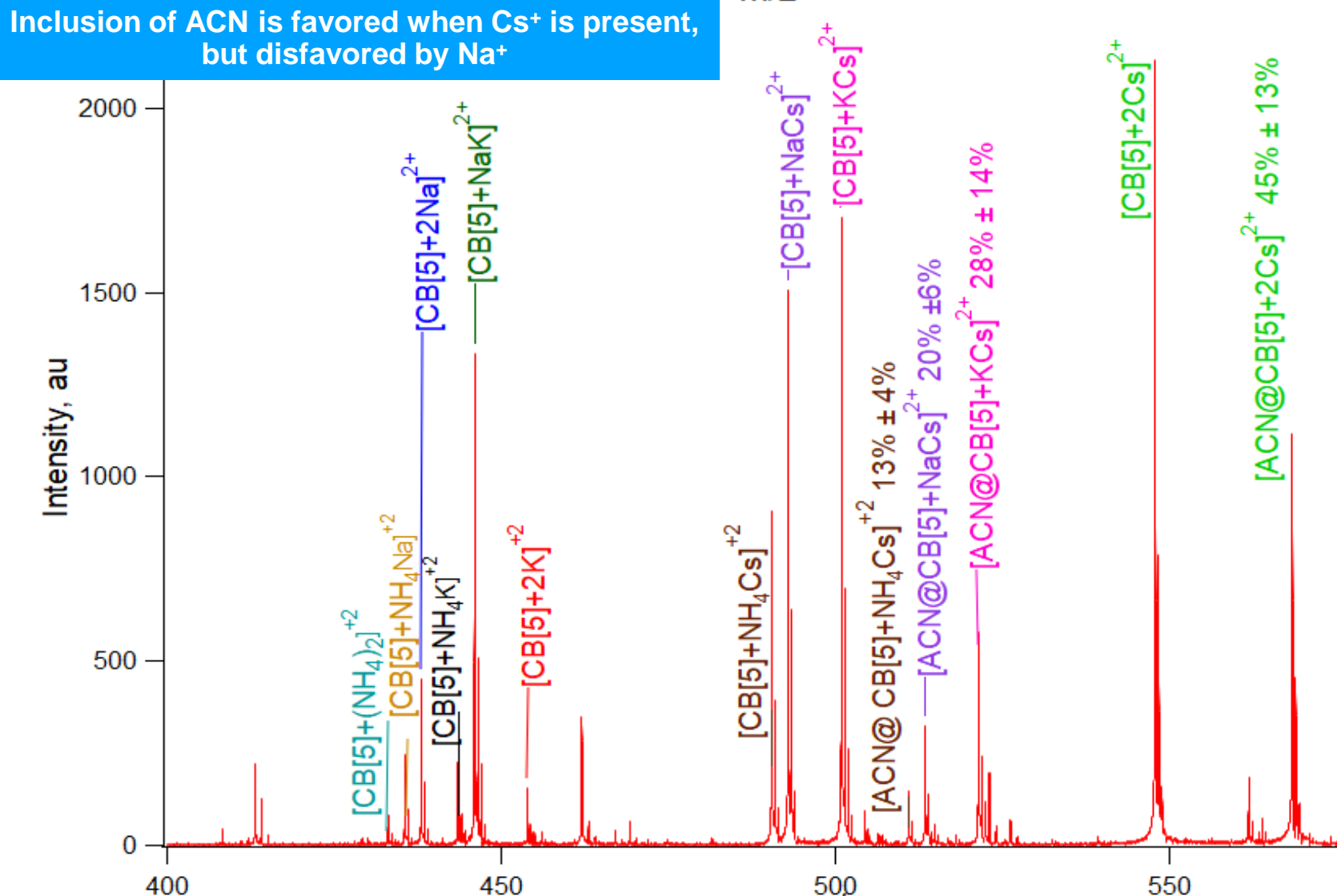
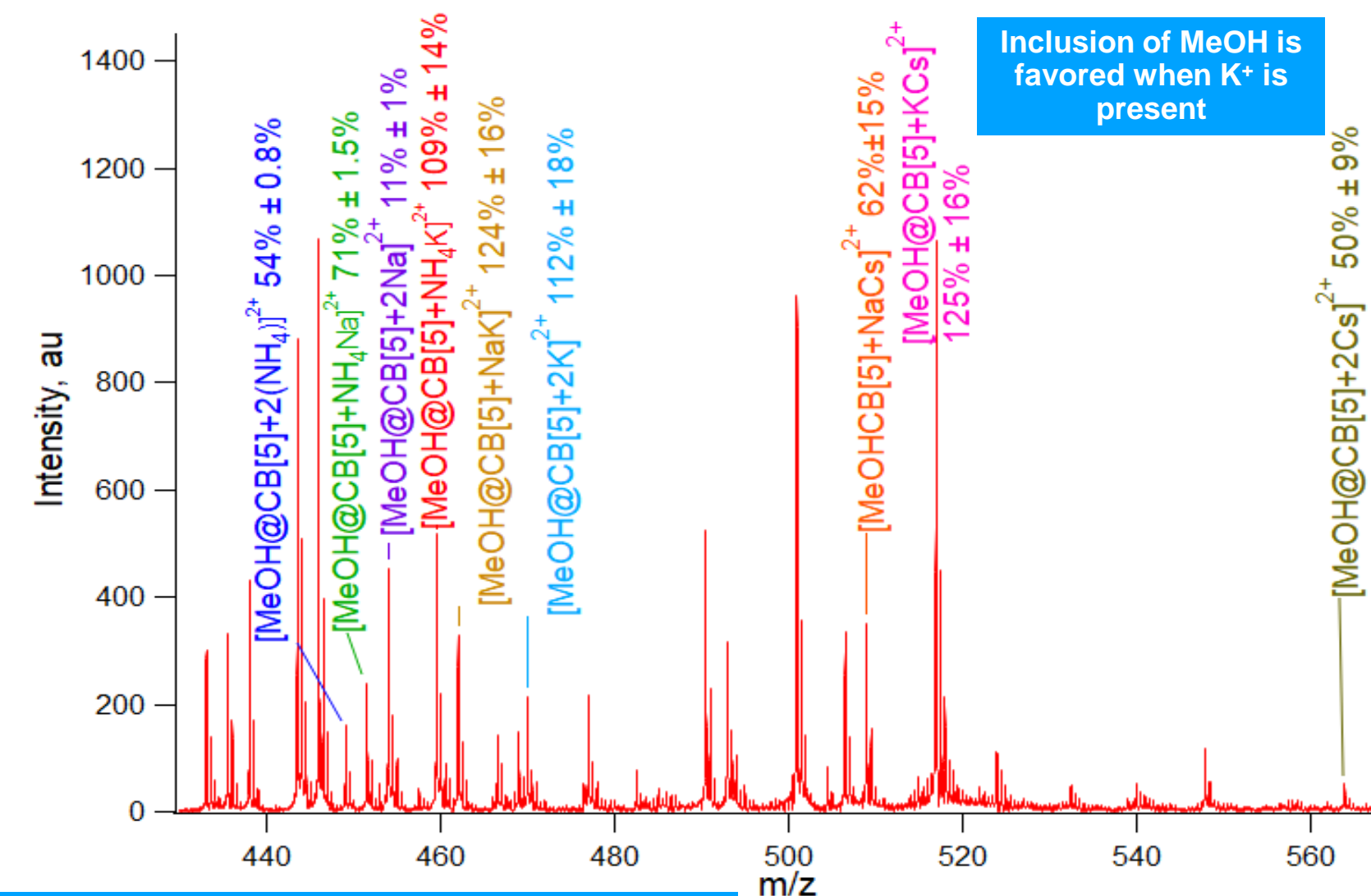
- 4.7 Tesla model APEX 47e Fourier transform ion cyclotron resonance mass spectrometer
- Electrospray ionization
- Modeling: Spartan '18 (MMFF94 force field)
- Host: Cucurbit[5]uril (CB[5])
- Guests: methanol, formic acid, and acetonitrile

Structure of CB[5] complexes

Methanol and formic acid easily fit inside the CB[5] cavity, but acetonitrile is so long it "bumps" the metal ions



Results: Metal-dependent guest binding; Size matters!



Conclusions

- Metal-dependent guest selectivity in CB[5] complexes is not based on the size of the metal or polarizability of the guest; it is based on "best fit" selectivity

Acknowledgments

- US National Science Foundation (Award # CHE-1904838)