

# Characterizations of tripeptides complexed with Zinc and Cadmium dications IRMPD

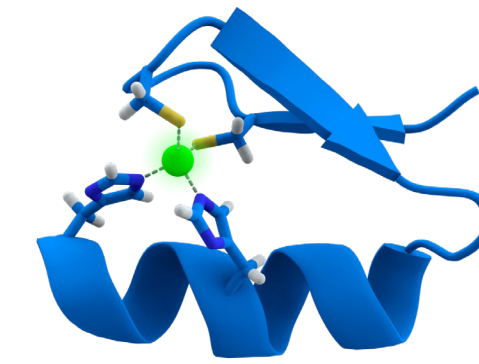


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## Introduction

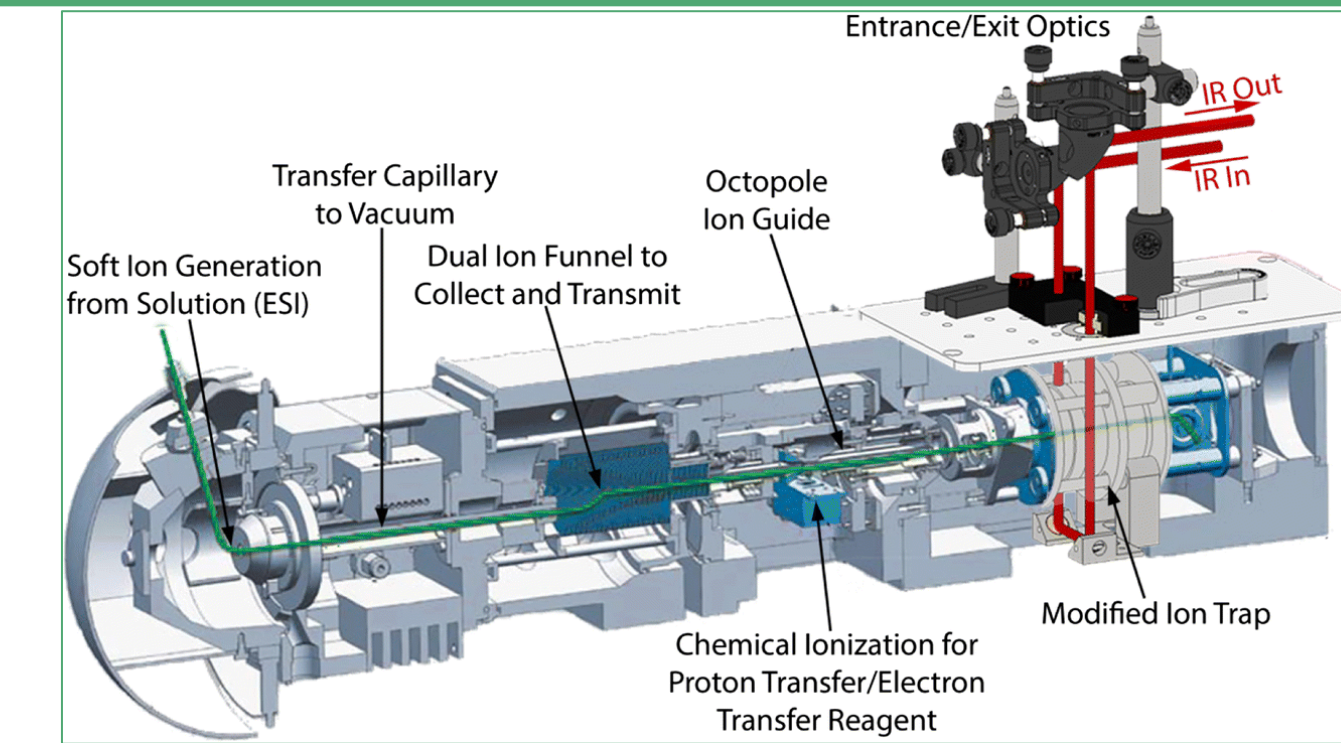
- Zinc plays a key role in structure and function in proteins (e.g. zinc fingers)
- Metalated amino acids can be studied in the gas phase to remove solvent-solute interactions
- Gas-phase complexes of the metalated tripeptides were investigated by infrared multiple photon dissociation (IRMPD) action spectroscopy using light generated from a free electron laser (FELIX).
- Ab initio* quantum chemical calculations were performed in parallel to identify several low-energy isomers for each complex and for comparison to the experimentally obtained spectra. These are listed below at B3LYP, B3LYP-GD3BJ, B3P86, and MP2(full) with 6-311+G(2d,2p) basis set.



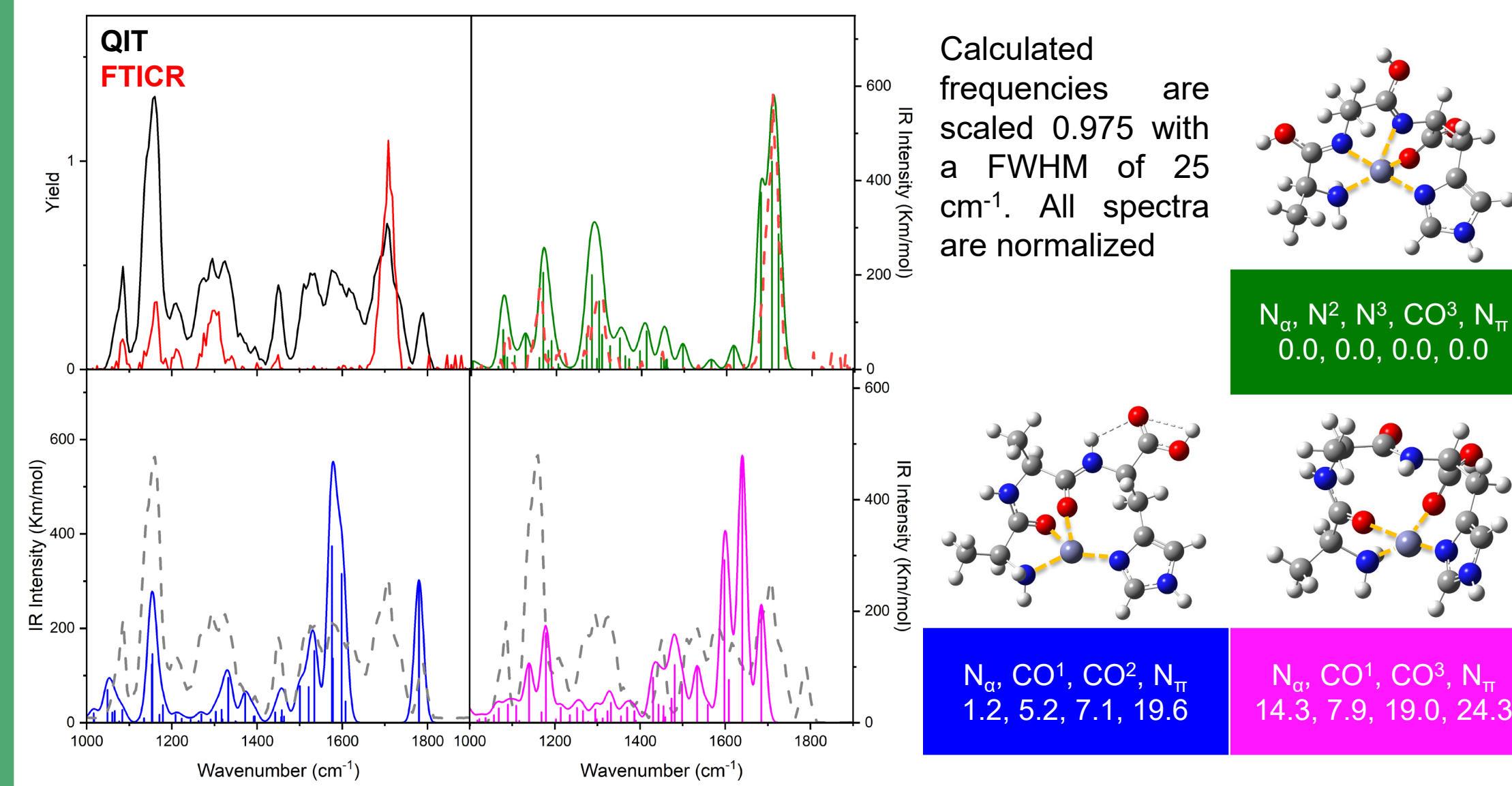
Zinc finger protein  
Zinc (green)  
coordinating with two  
His and two Cys  
residues

## Instrumentation

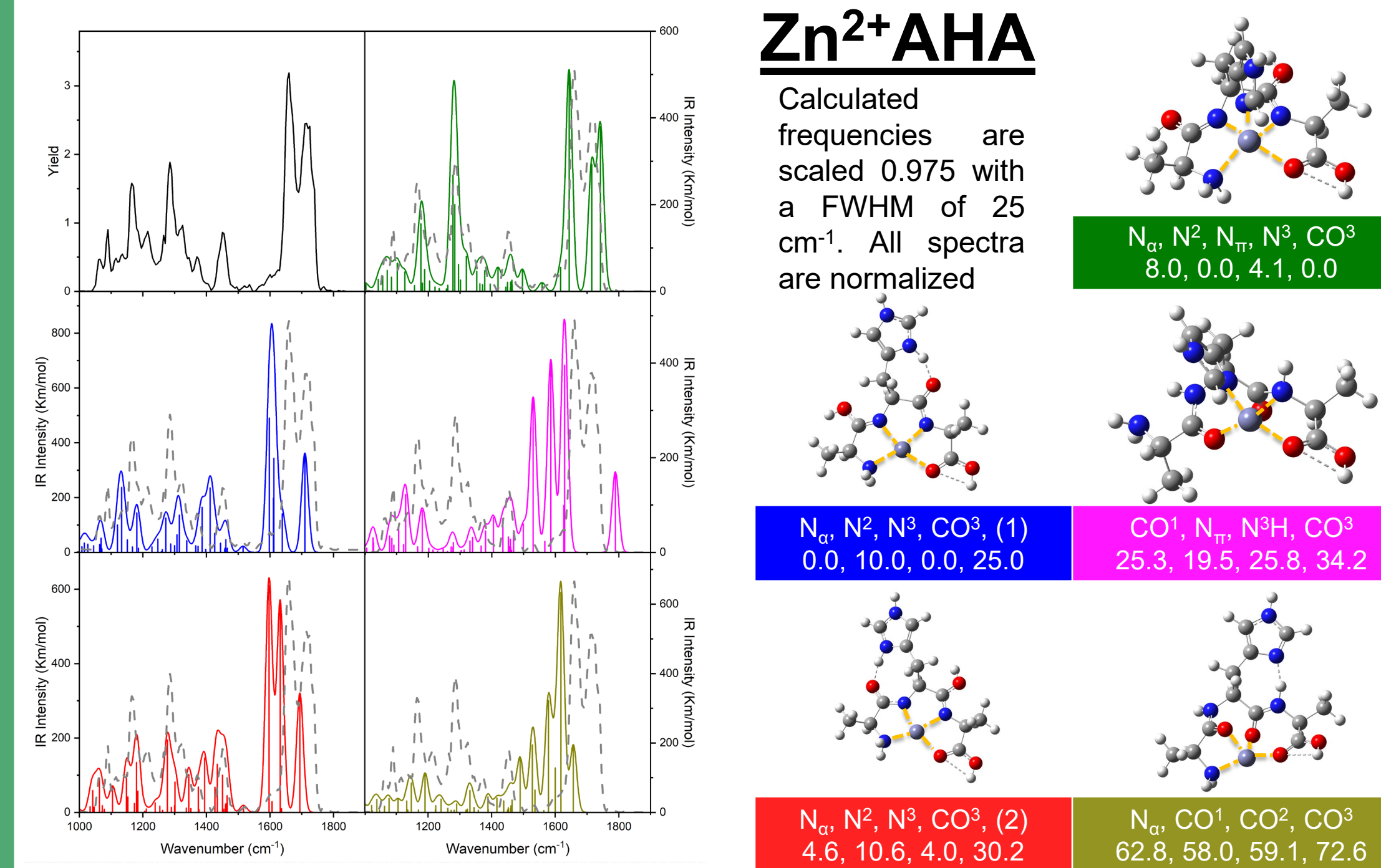
- Ions are generated and trapped
- Trapped ions are irradiated
- Resonant absorption of light causes photodissociation
- Plotting the fragment fluence as a function of wavelength allows comparison to simulated spectra from calculations



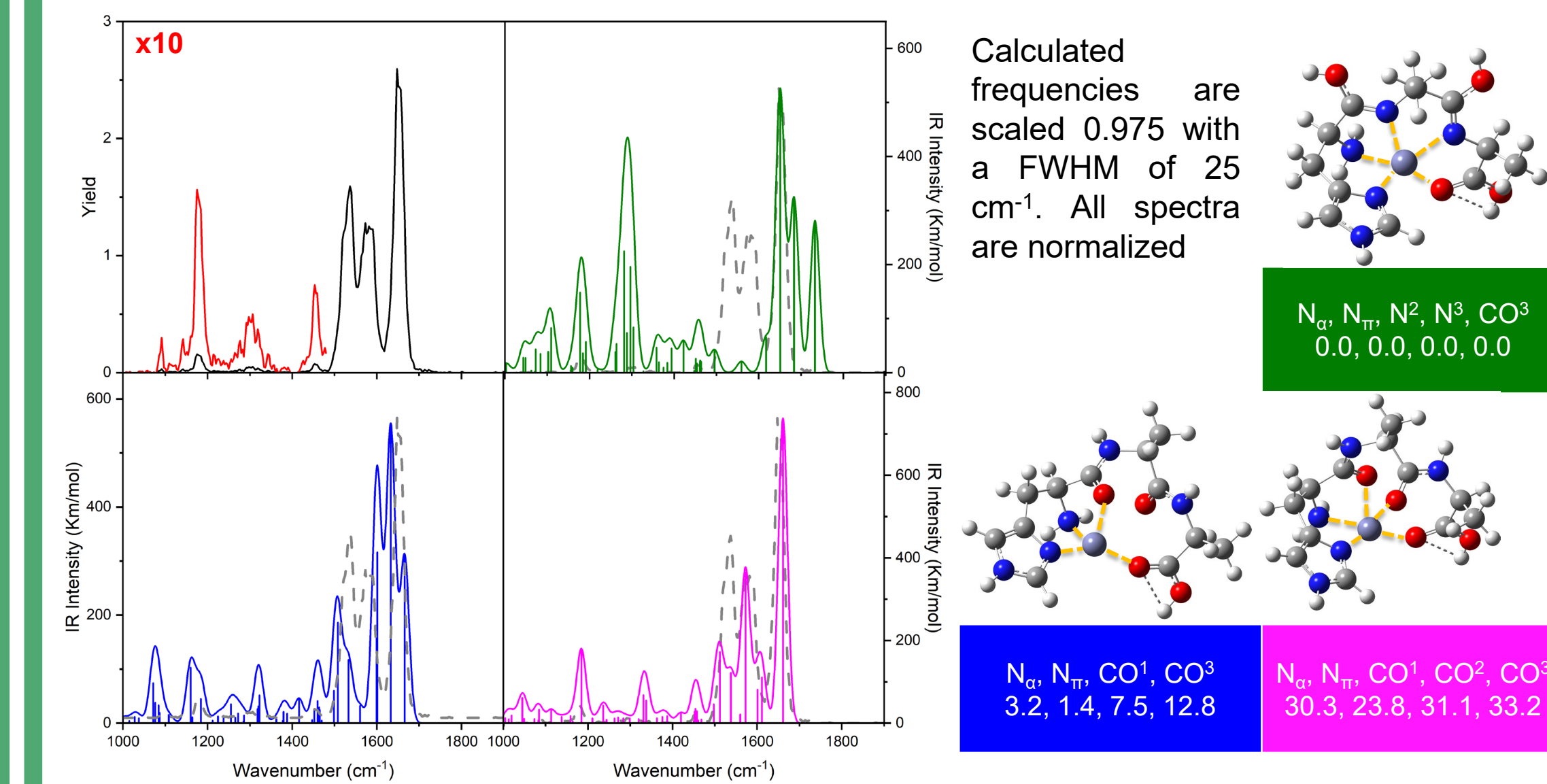
## Zn<sup>2+</sup>AAH



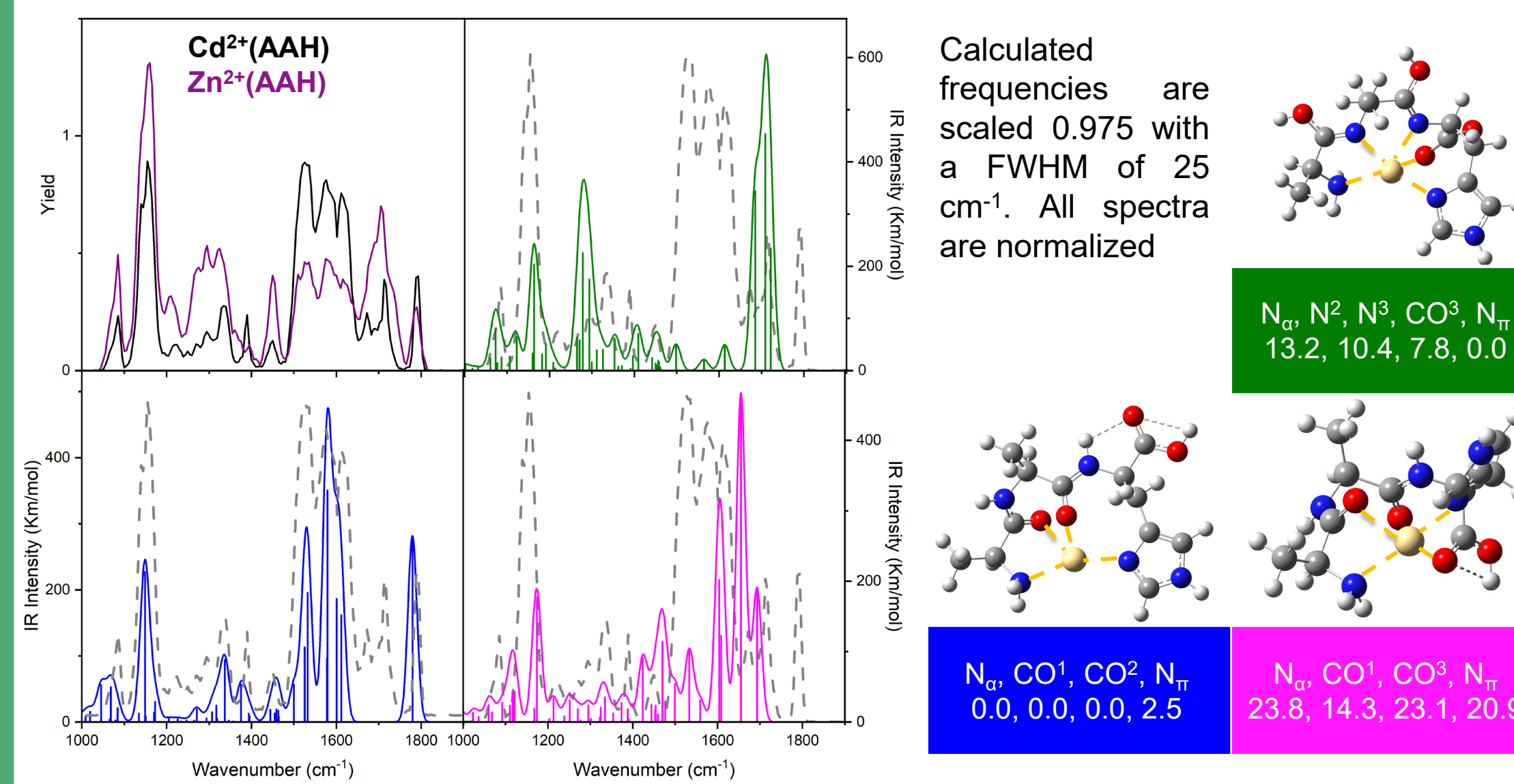
## Zn<sup>2+</sup>AHA



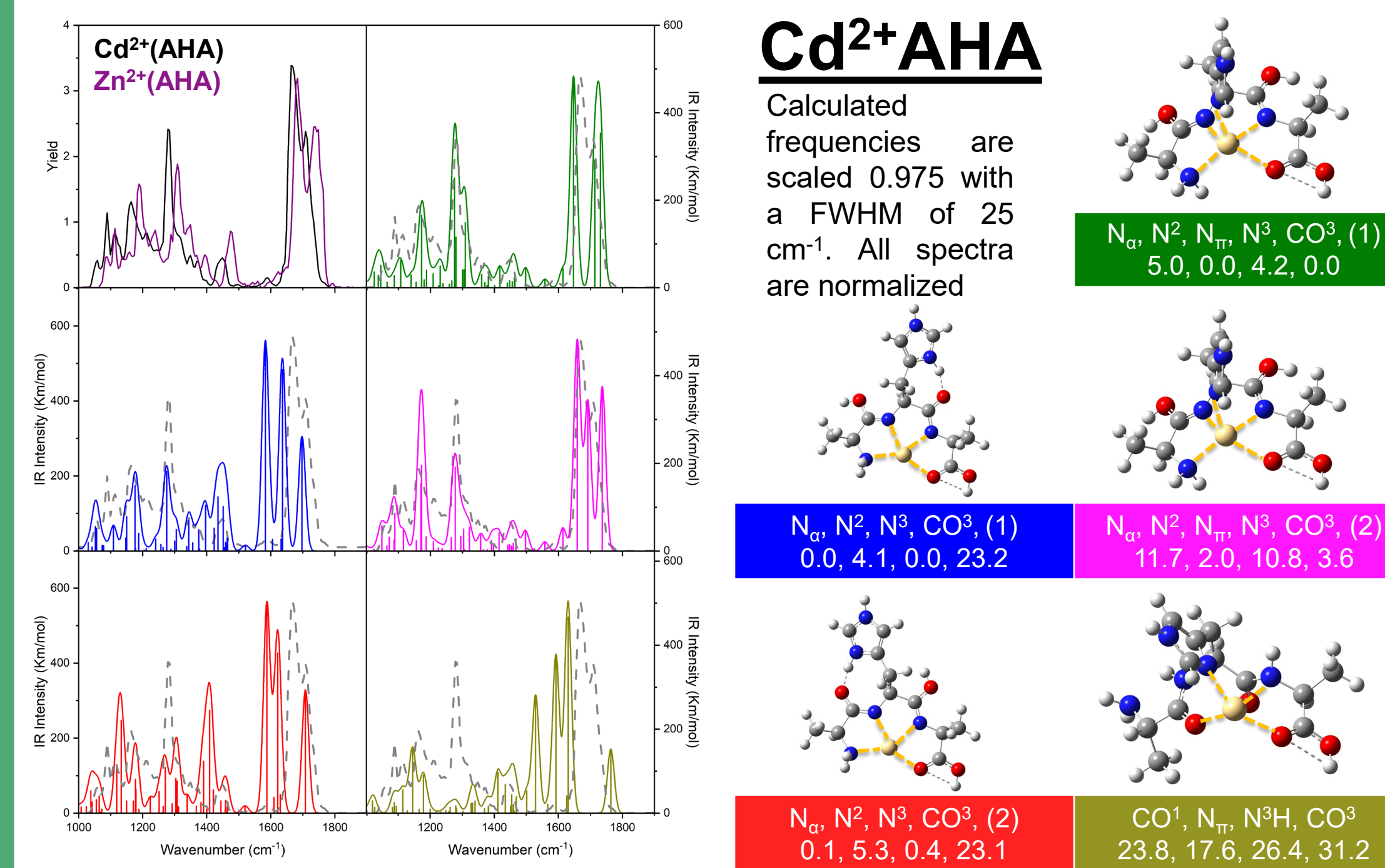
## Zn<sup>2+</sup>HAA



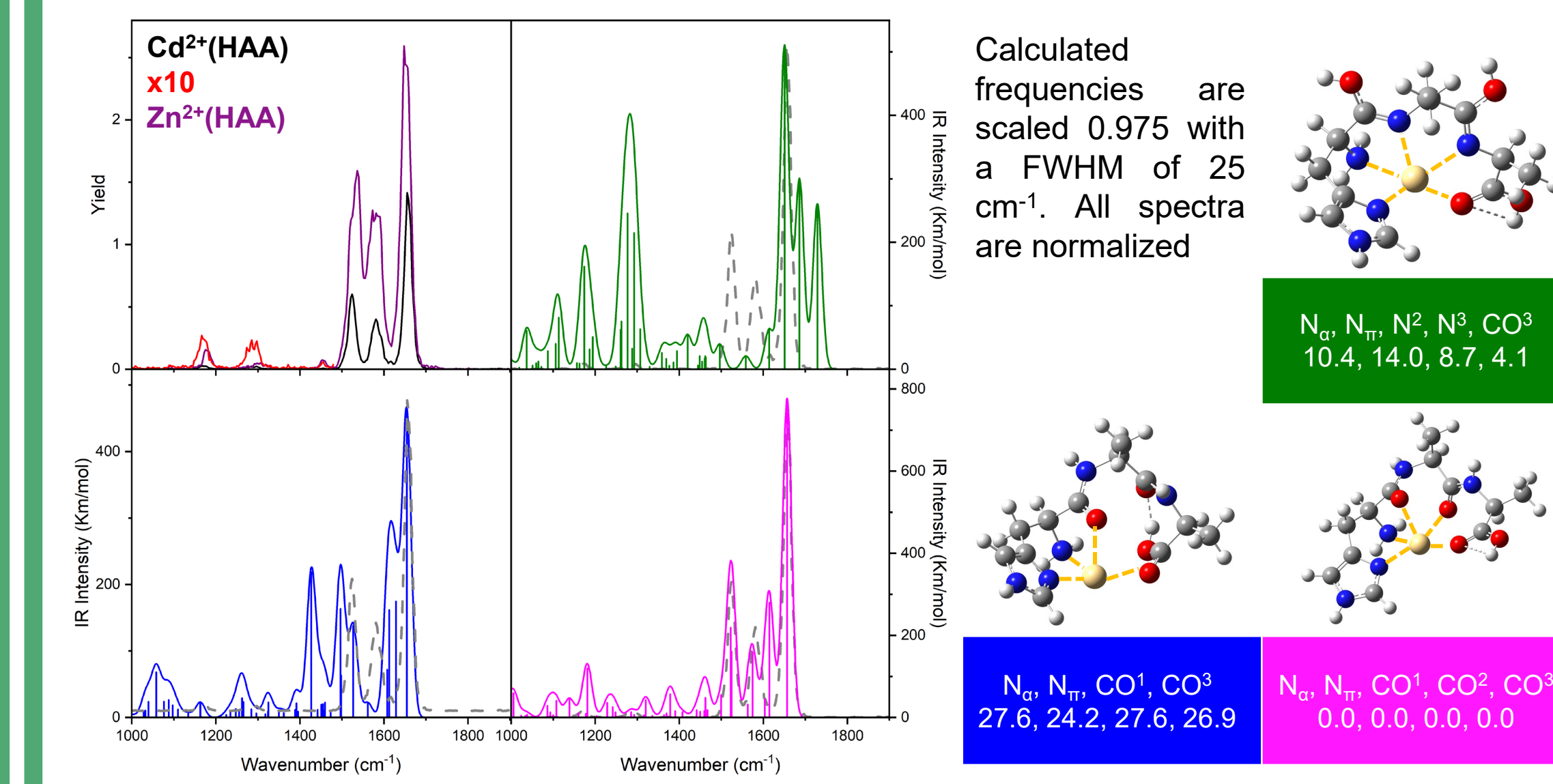
## Cd<sup>2+</sup>AAH



## Cd<sup>2+</sup>AHA



## Cd<sup>2+</sup>HAA



## Acknowledgements

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