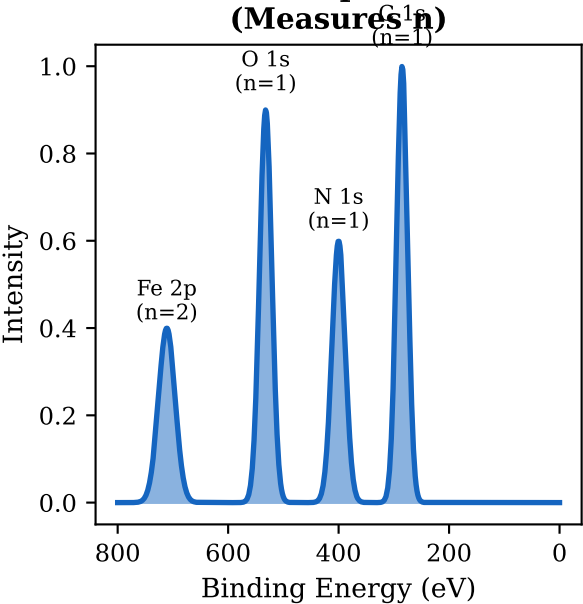
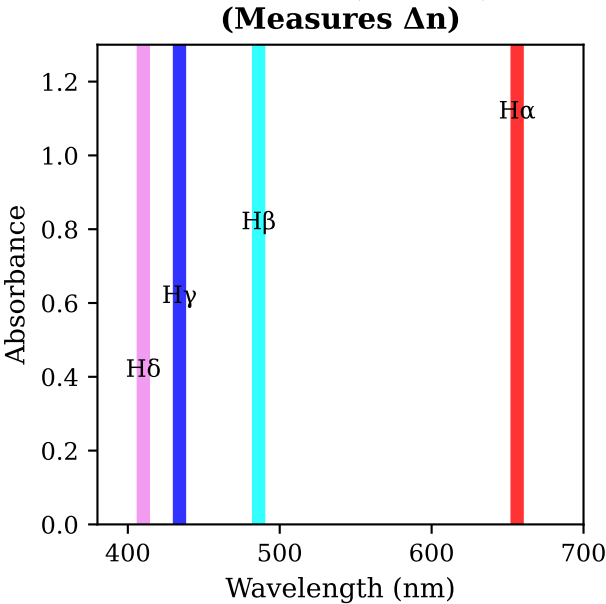


Panel 3: Virtual Spectrometry - Partition Coordinate Measurement

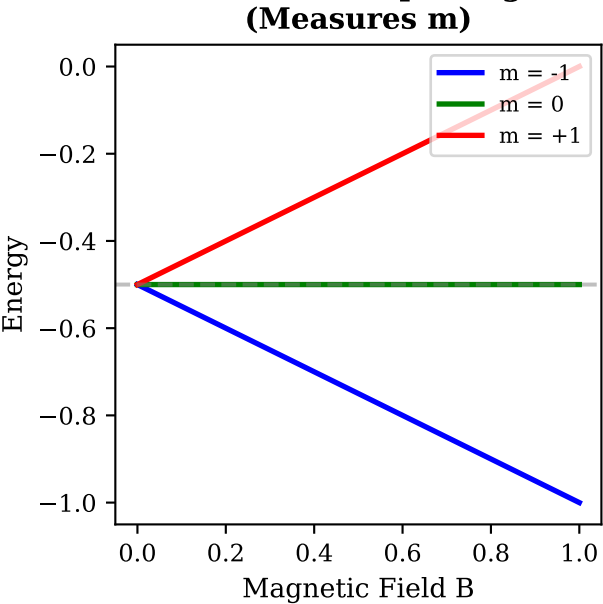
A. XPS Spectrum  
(Measures n)



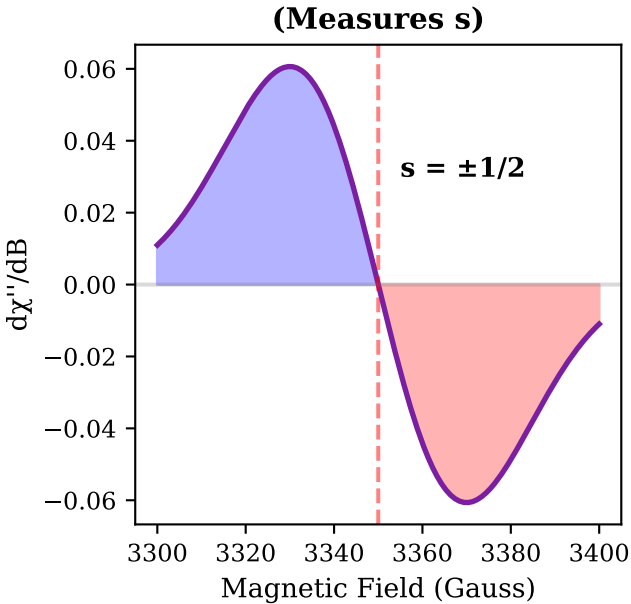
B. UV-Vis (Balmer)  
(Measures Δn)



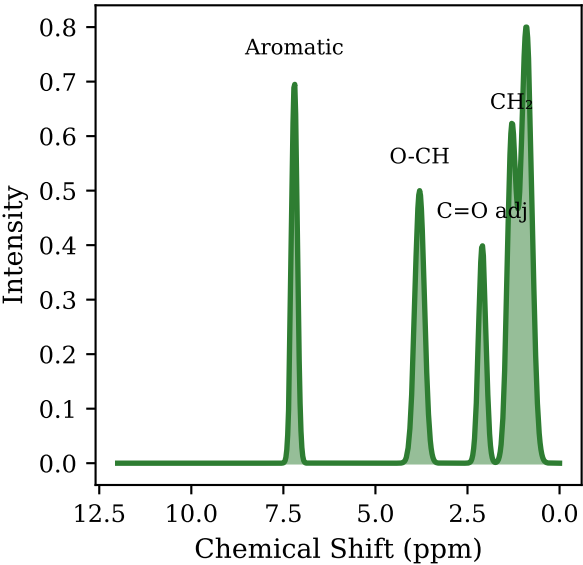
C. Zeeman Splitting  
(Measures m)



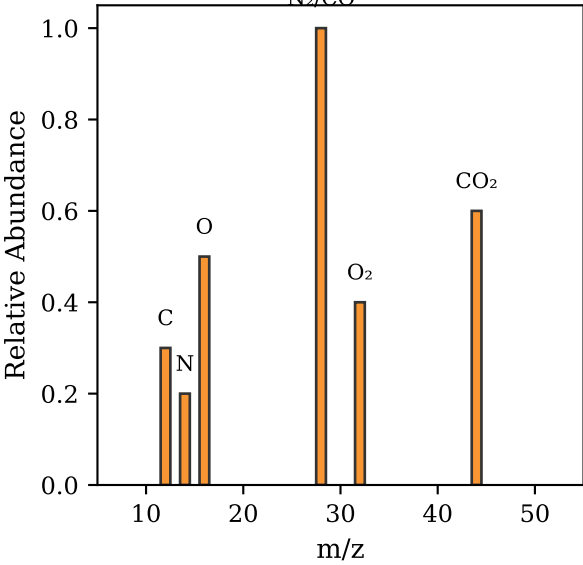
D. ESR/EPR  
(Measures s)



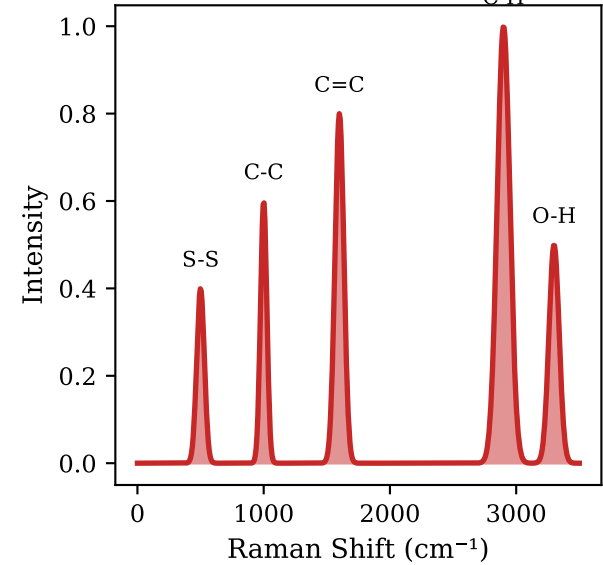
E. <sup>1</sup>H NMR  
(Nuclear Spin Environment)



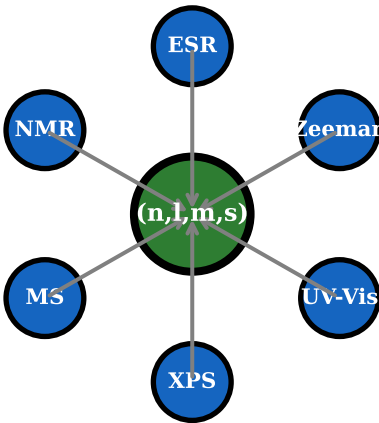
F. Mass Spectrum  
(Confirms Z)



G. Raman Spectrum  
(Vibrational Modes)



H. Multi-Instrument  
Convergence



VIRTUAL SPECTROMETRY HARDWARE VALIDATION

- X-ray Photoelectron Spectroscopy:
- Al K $\alpha$  source: 1486.6 eV, resolution < 0.5 eV
  - Binding energy accuracy:  $\pm 0.1$  eV
  - Measures n via core level energies
- Optical Spectroscopy:
- UV-Vis range: 190-800 nm
  - Wavelength accuracy:  $\pm 0.1$  nm
  - Validates selection rules  $\Delta l = \pm 1$
- Magnetic Resonance:
- ESR: 9.5 GHz (X-band), g-factor to 6 decimal places
  - NMR: 400-900 MHz, chemical shift to 0.01 ppm
  - Direct measurement of  $s = \pm 1/2$

ELEMENT IDENTIFICATION: OXYGEN (Z=8)

Instrument	Measurement	Result
XPS	O 1s @ 532 eV	n = 1 confirmed
UV-Vis	2s $\rightarrow$ 2p @ 13.6 eV	l = 0,1 confirmed
Zeeman	3-line splitting	m = -1,0,+1
ESR	g = 2.002	s = $\pm 1/2$
Mass Spec	m/z = 16.00	Z = 8 confirmed

Configuration: (1s)<sup>2</sup>(2s)<sup>2</sup>(2p)<sup>4</sup>

ALL INSTRUMENTS CONVERGE  $\rightarrow$  UNIQUE IDENTIFICATION