The visible spectrum of iridium monohydride and monodeuteride

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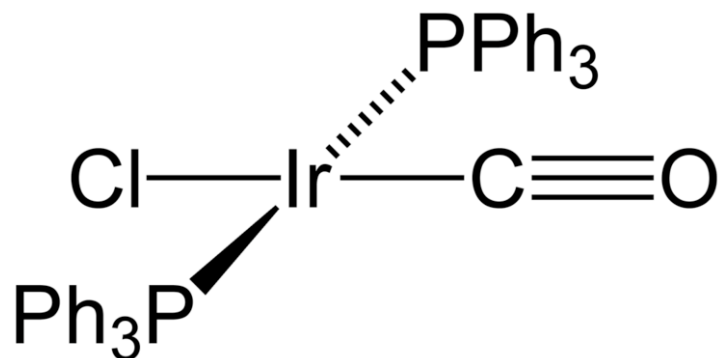C. LINTON AND D. W. TOKARYK, Physics Department, and Centre for Lasers, and Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, NB, E3B 5A3

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UNB

Why should we study diatomic species?

Change in electronic character as a function of changing ligand or transition metal

Comparisons between theory and experiment

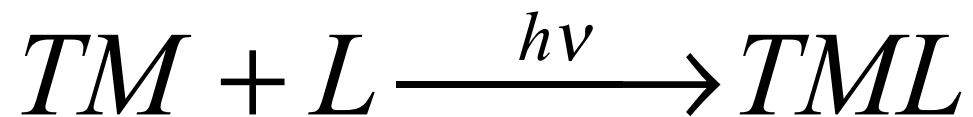Transition metal complexes important catalytically

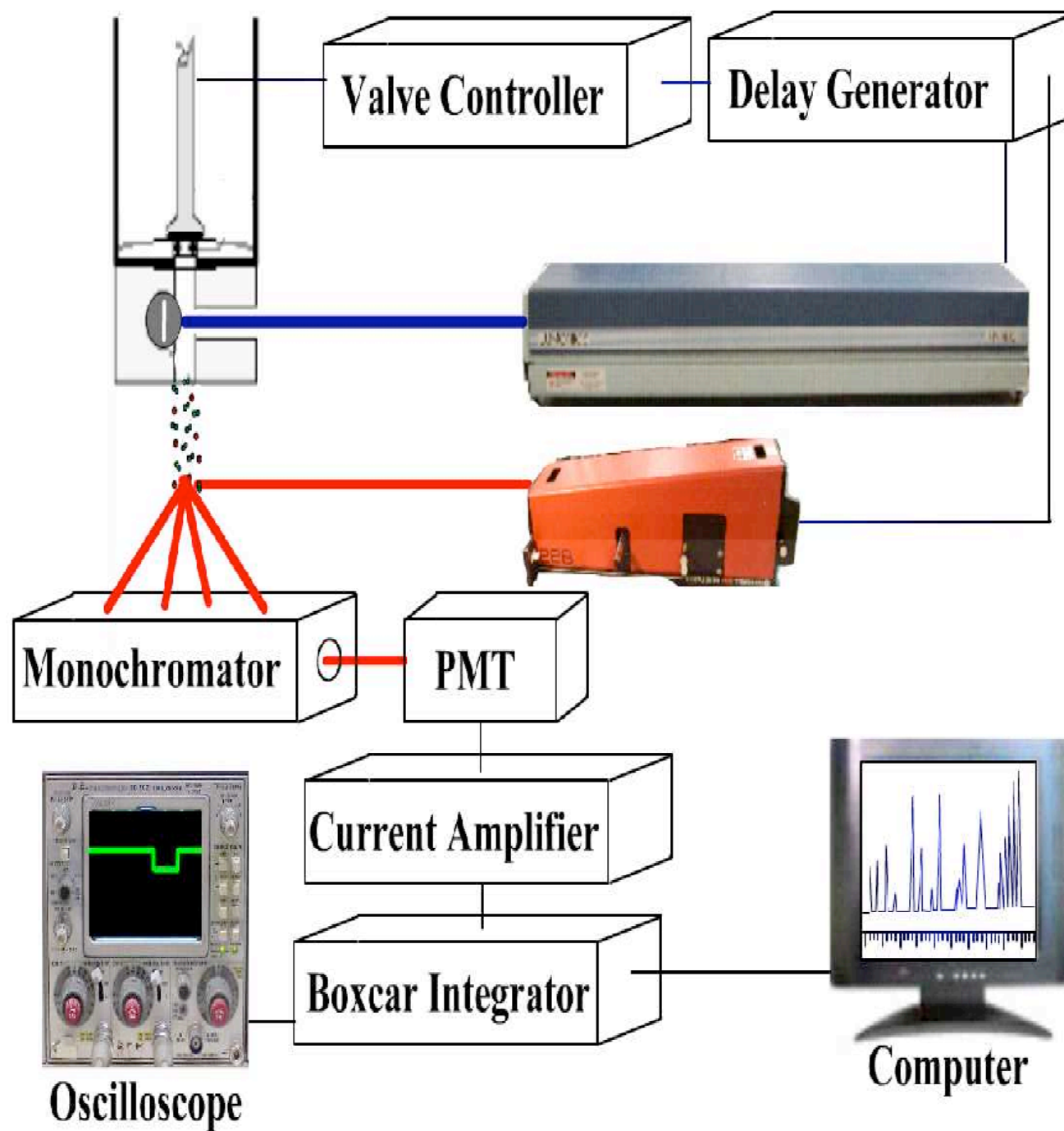# Iridium monohydride and monodeuteride - IrH/IrD

Motivations

- Prior work – no experimental studies
- Only five iridium-containing diatomics published to date

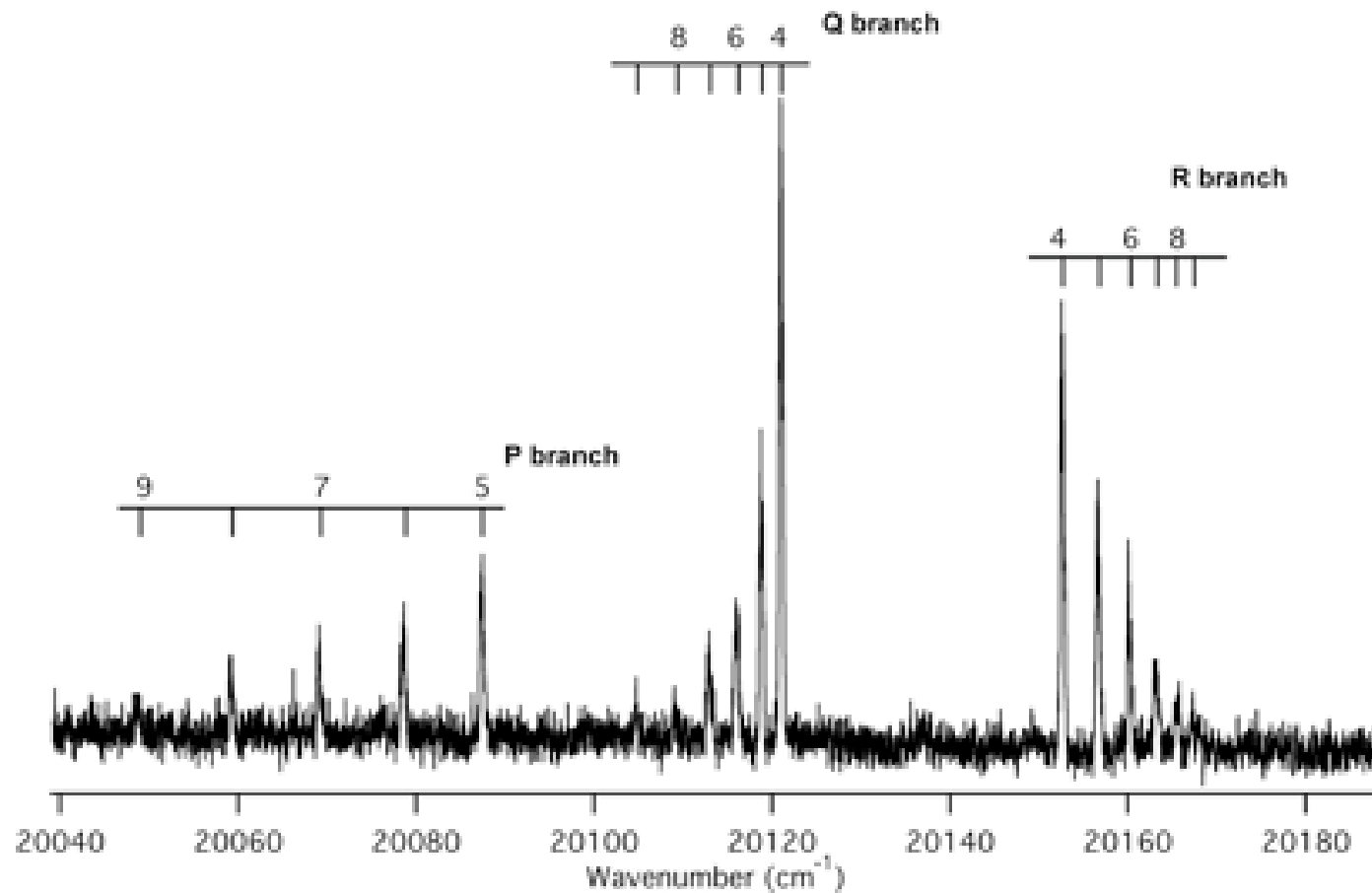- Continues work on group 9-monohydrides (CoH, RhH, and IrH)

Synthesis of Diatomic Species

- Transition-metal source (metal rod)
- Reactant Source (reactant gas)
- Heat (UV laser)

$$TM + L \xrightarrow{\ h\nu\ } TML$$

Valve Controller

Delay Generator

Monochromator

PMT

Current Amplifier

Boxcar Integrator

Oscilloscope
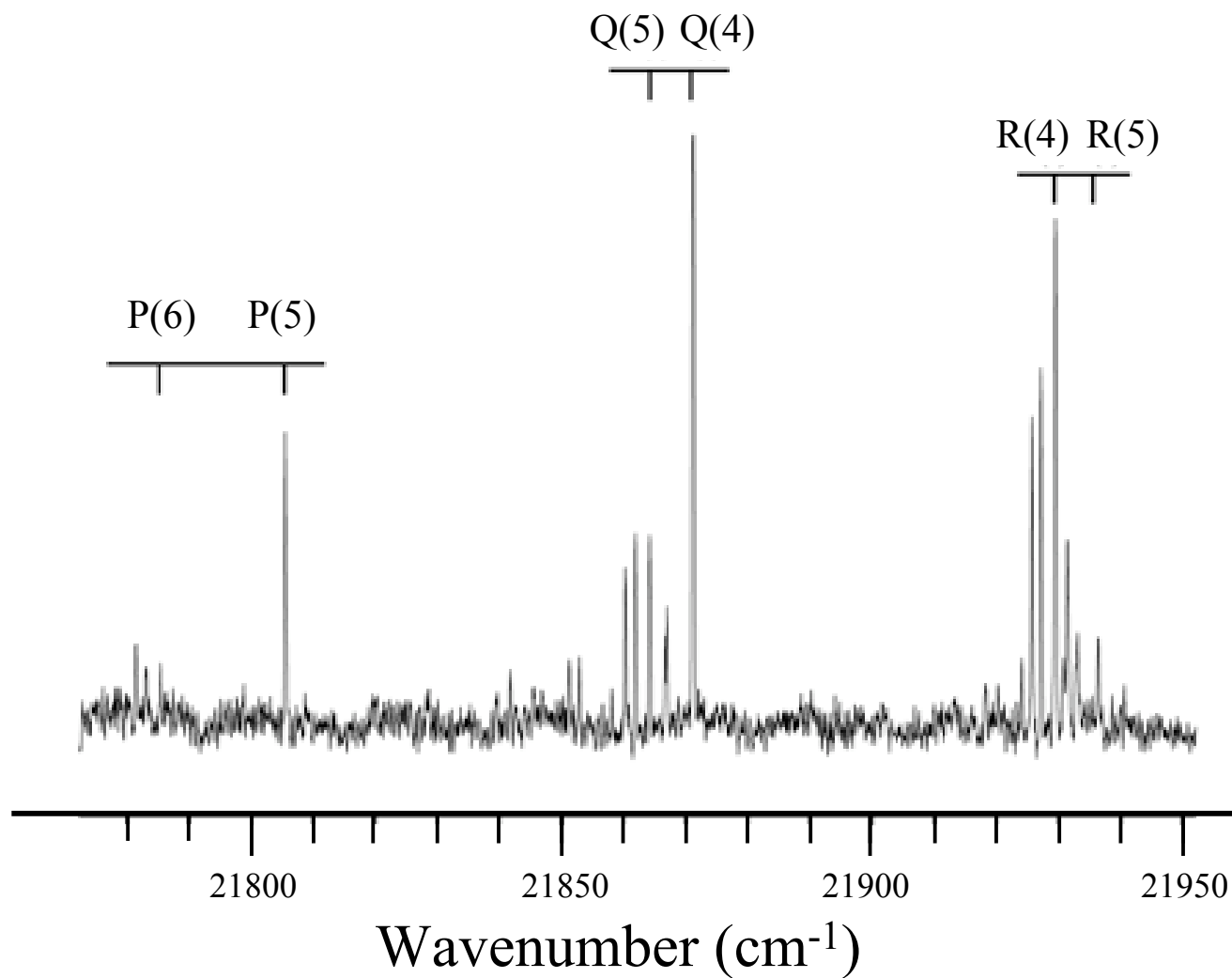
Computer

5

Low resolution (IrD)
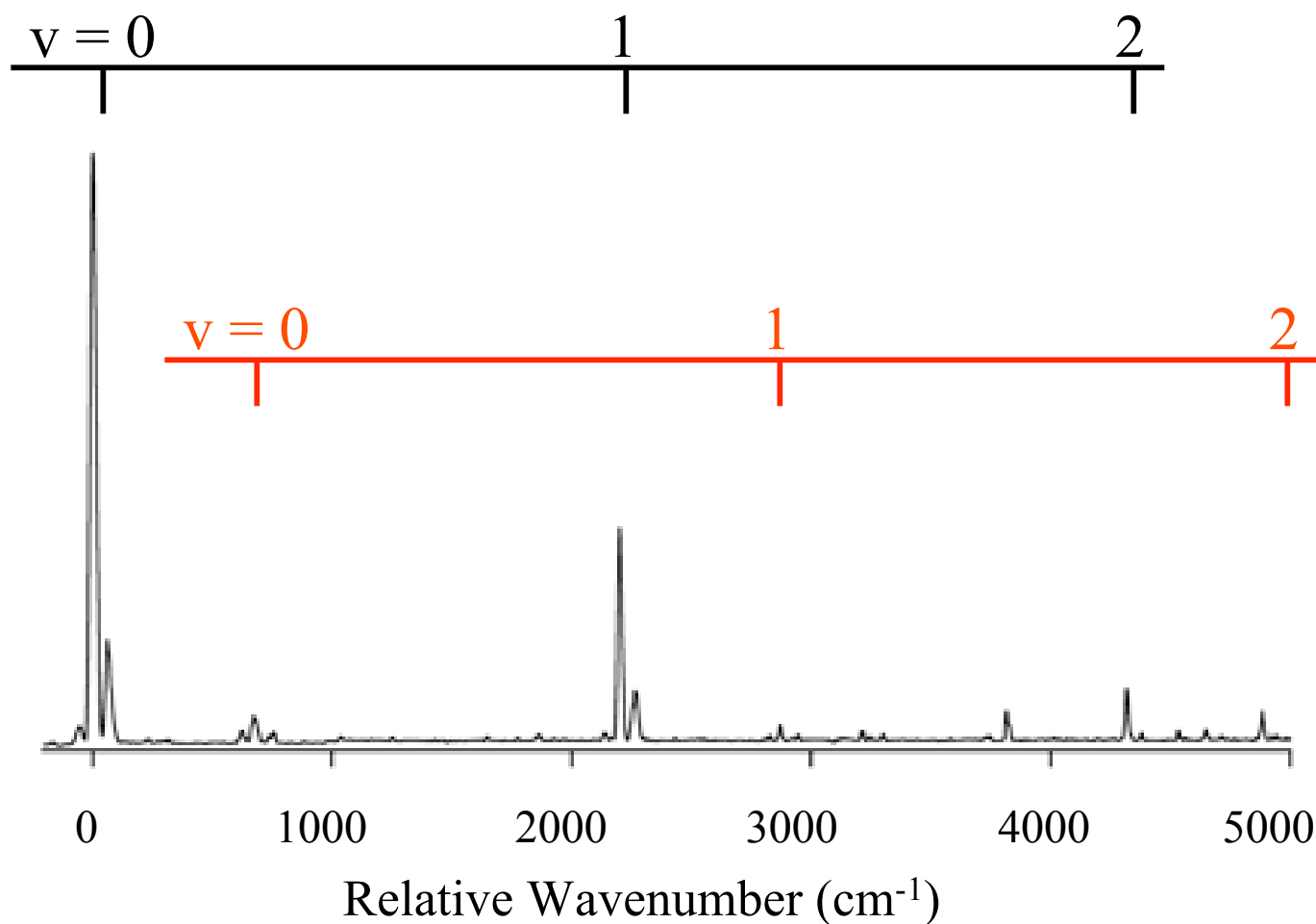
Determination of the ground state of IrH/IrD

- First lines R(4), Q(4), P(5)

- CoH ($^3\Phi_i$) [Bernath (1996)], CoF ($^3\Phi_i$) [Adam (1994)],, IrF ($^3\Phi_i$) [Adam (2009)],

- Theory predicts either $^3\Delta$ [Cassarubios (1999), Wittborn (1995)] or $^3\Sigma^-$ [Balasubramanian (1991)]

- All studies predict a low-lying $^3\Phi$ state

$$^3\Phi_4$$

Low resolution (IrH) with 'extra' lines

Q(5) Q(4)

R(4) R(5)

P(6)   P(5)

21800   21850   21900   21950

Wavenumber (cm^{-1})

Dispersed fluorescence of 553 nm band of IrH

Vibrational Analysis

	Vibrational frequency (cm^{-1})	Anharmonicity term (cm^{-1})
IrH G.S.	2140(11)	--
IrH low-lying	~ 2100	--
IrD G.S.	1609(2)	19.3(5)
IrD low-lying	~ 2100	--

Rotational fit results

Molecule	Assignment	T (cm^{-1})	B (cm^{-1})	D (cm^{-1}) x 10^{-3}
IrH	X$^3\Phi_4$ v=0	0 fixed	6.540(4)	0.25 fixed
		18060.3(3)	6.67(3)	6.1(7)
		18459.2(3)	6.31(3)	4.4(7)
		19720.7(3)	6.89(3)	12.7(6)
		20488.3(2)	6.24(6)	--
		21189.9(3)	6.33(3)	11.1(7)
		21873.5(2)	5.88(1)	--
		22555.4(3)	6.17(3)	8.4(7)
		23466.4(2)	6.57(1)	--

Comparison with RhH and CoH

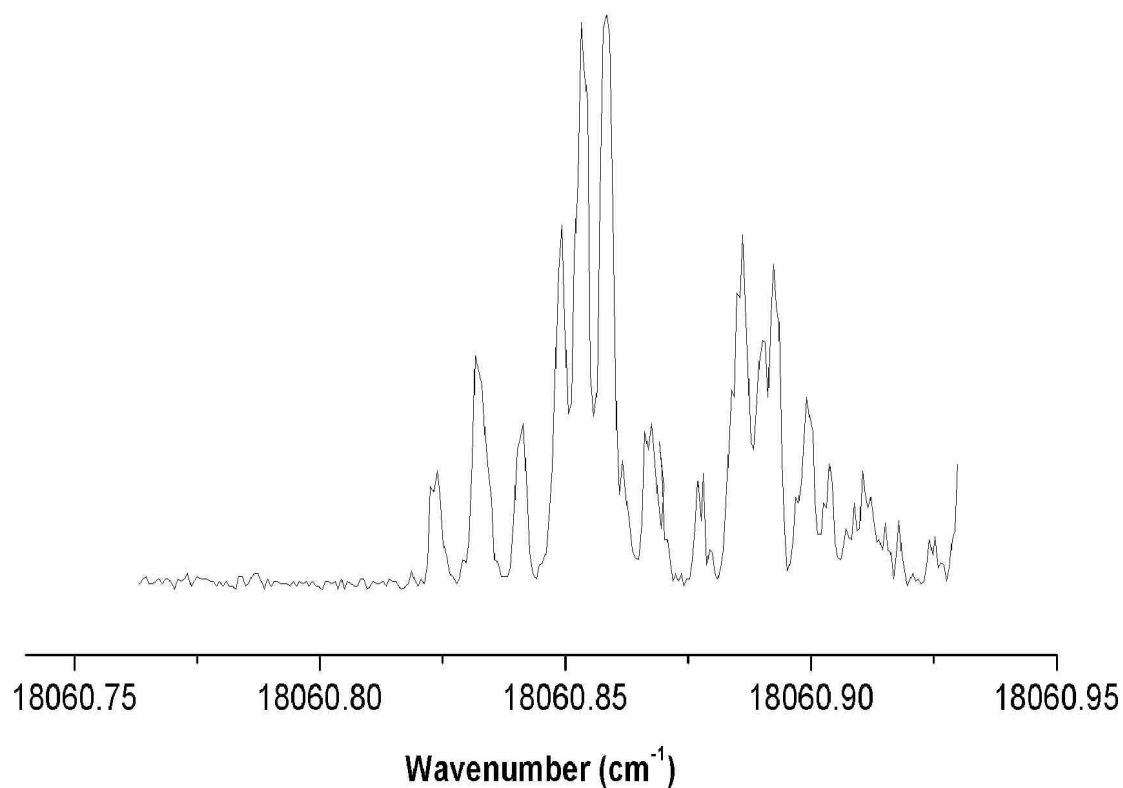| Parameter	B (cm^{-1})	r (Å)	ω_e (cm^{-1})	k (N/m)
CoH[1]	7.14	1.53	1859	202
RhH[2]	6.55	1.59	2040	245
IrH	6.54	1.60	2140	271

[1]Bernath 1996

[2]Balfour 2000

High resolution at UNB, Q(4) line
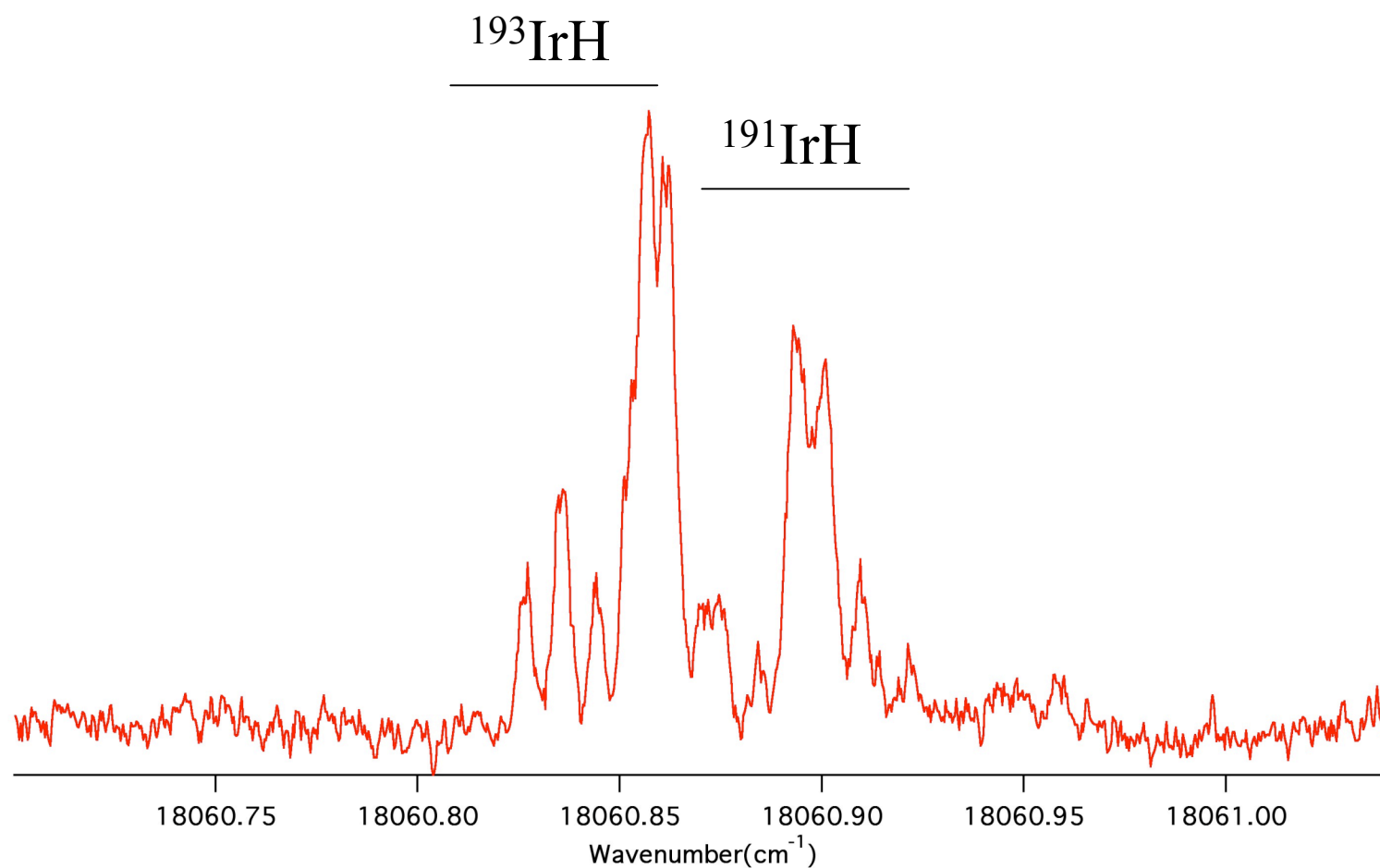
High resolution at Arizona State University (Steimle Lab), Q(4) line

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Questions?