High Precision Spectroscopy of ^{177}HfF$^+$ and ^{179}HfF$^+$
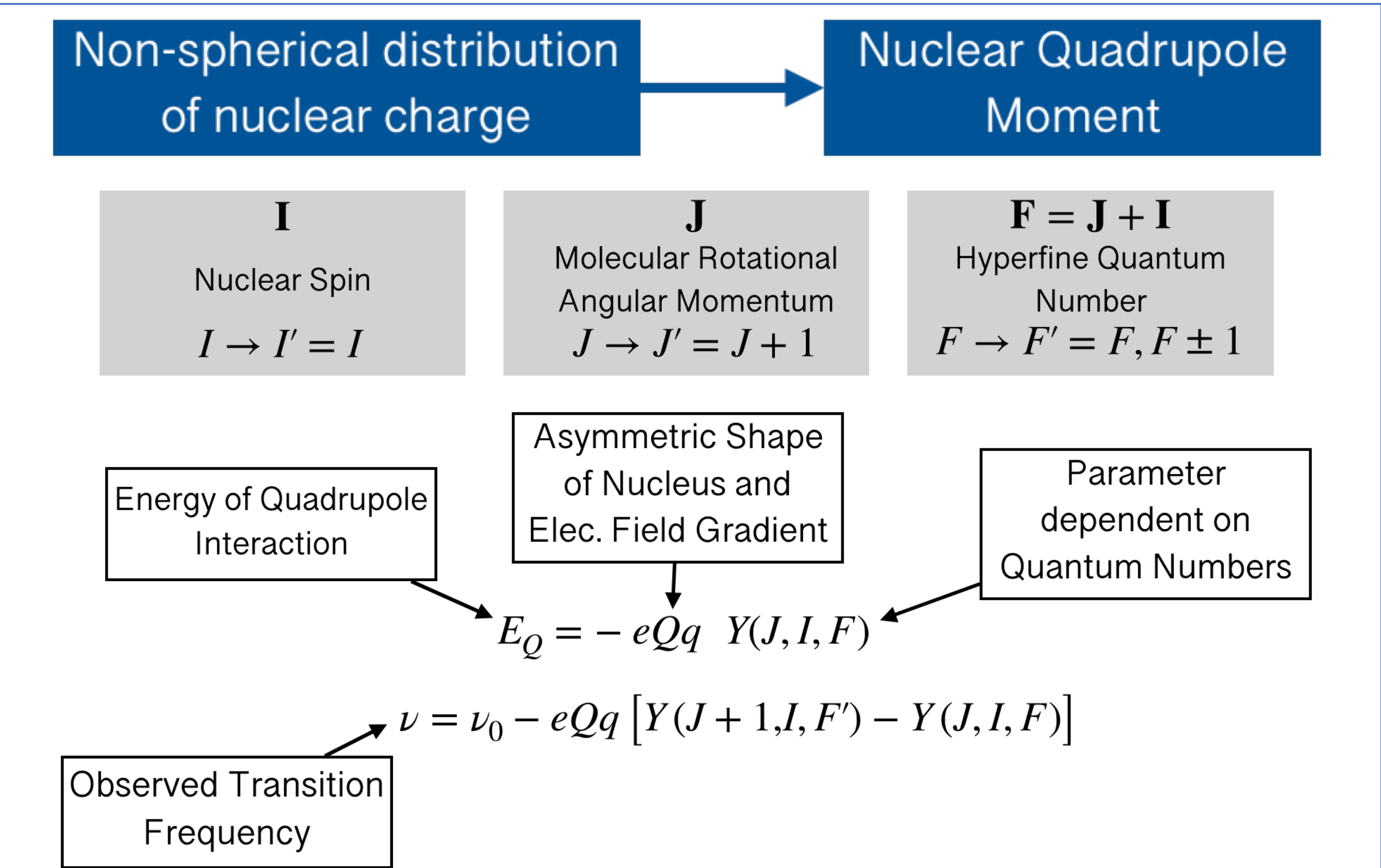
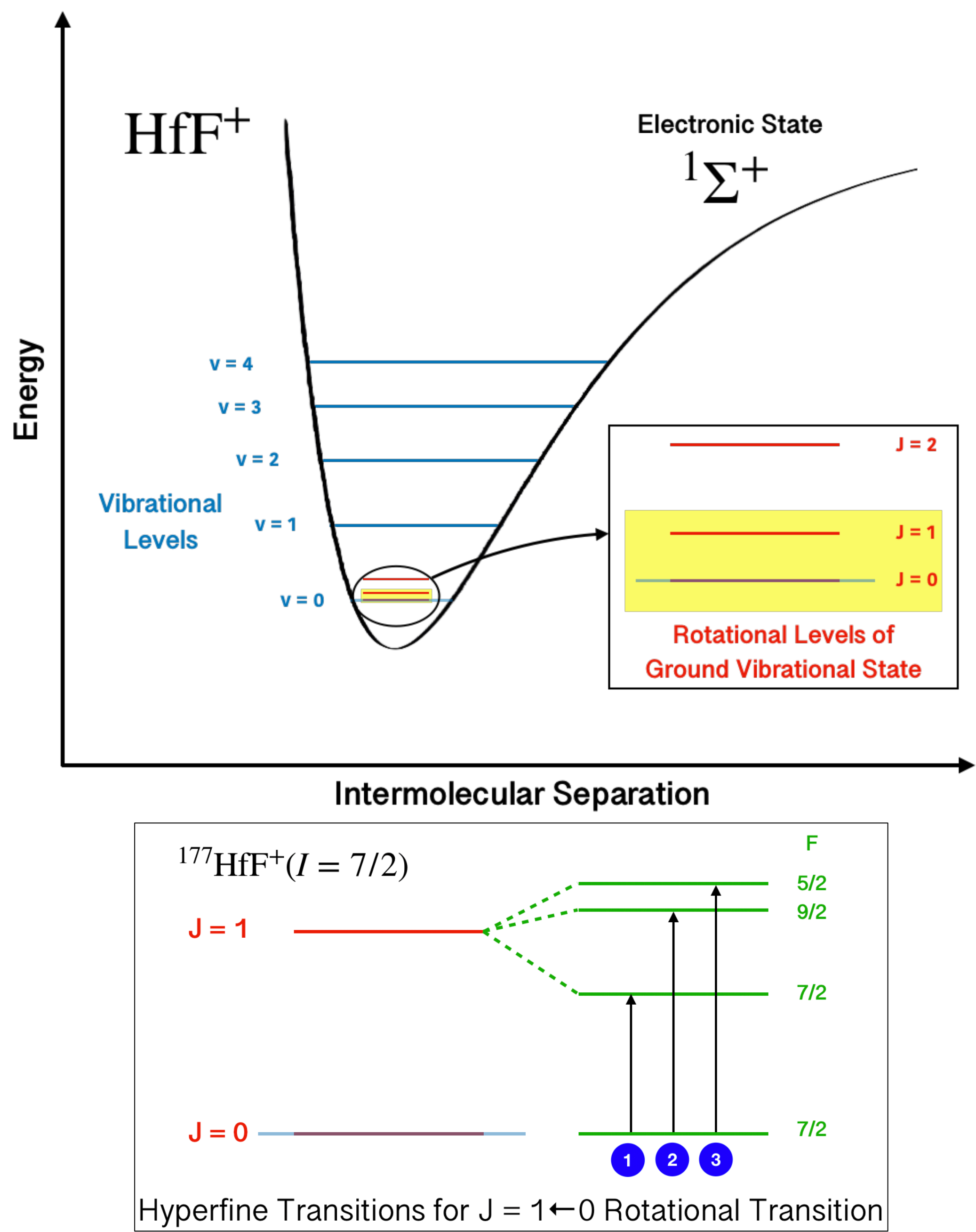## William R. Ballard and Richard J. Mawhorter
Pomona College, Claremont, CA, USA

Introduction

- Theorists have identified the odd isotopologues of HfF$^+$ as optimal testing grounds for **parity non-conserving** effects [1].

- Eric Cornell's group at JILA in Boulder, CO has selected ^{180}HfF$^+$ as its molecule to search for the electron electric dipole moment (eEDM) [2].

- In support of these efforts, I calculated the $J = 1 \leftarrow 0$ hyperfine transitions in ground vibrational state of ^{177}HfF$^+$ and ^{179}HfF$^+$.

- The aim of the predictions is to facilitate the measurement of these transitions, which would help determine essential quantities (e.g. electric field gradient at the nucleus).
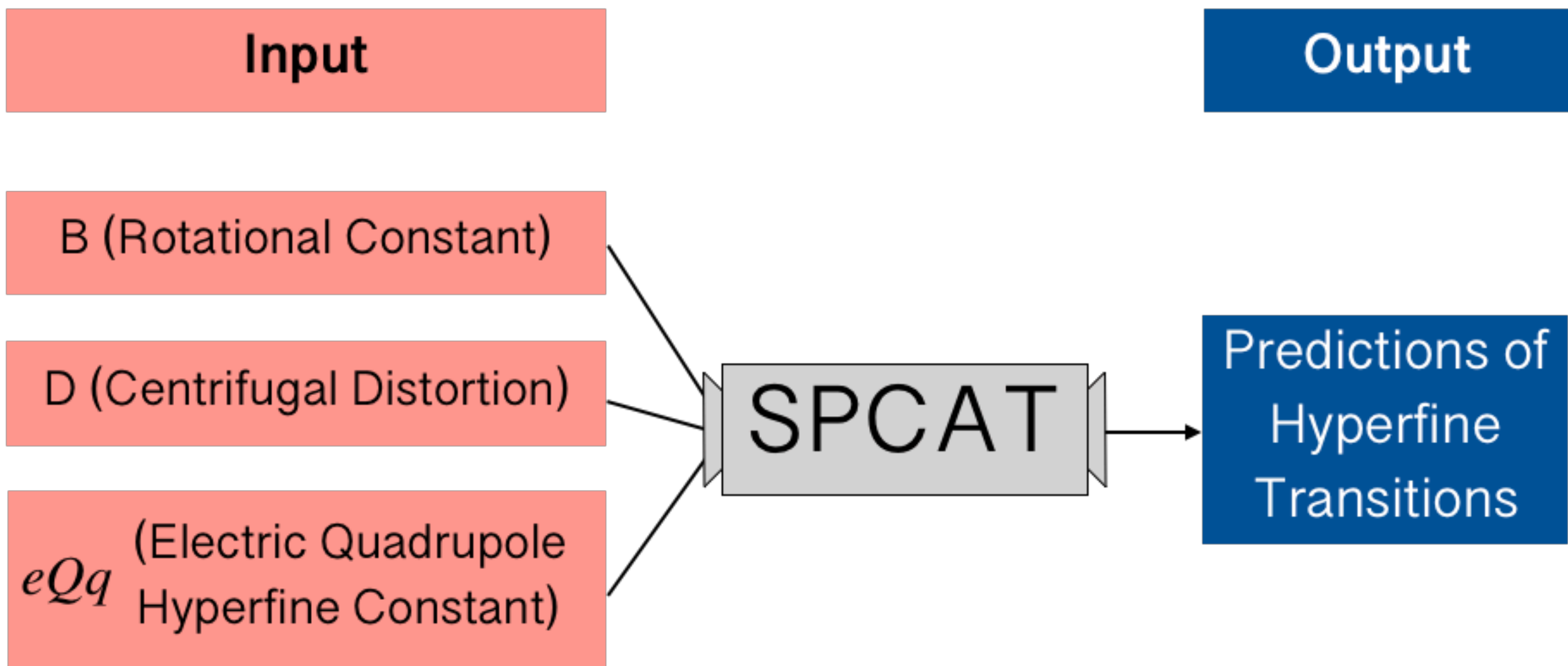
Theory of Quadrupole Splitting

| Non-spherical distribution of nuclear charge | → | Nuclear Quadrupole Moment |

I	**J**	**F = J + I**
Nuclear Spin	Molecular Rotational Angular Momentum	Hyperfine Quantum Number
$I \rightarrow I' = I$	$J \rightarrow J' = J + 1$	$F \rightarrow F' = F, F \pm 1$

Energy of Quadrupole Interaction — Asymmetric Shape of Nucleus and Elec. Field Gradient — Parameter dependent on Quantum Numbers

$$E_Q = -eQq \ Y(J, I, F)$$

$$\nu = \nu_0 - eQq \left[Y(J+1, I, F') - Y(J, I, F) \right]$$

Observed Transition Frequency

Rotational levels will split due to quadrupole interaction [3].

HfF$^+$

Electronic State $^1\Sigma^+$

Rotational Levels of Ground Vibrational State

^{177}HfF$^+(I = 7/2)$

Hyperfine Transitions for $J = 1 \leftarrow 0$ Rotational Transition

Computational Method

- I used the SPCAT package by Pickett [3] to calculate frequency of desired transitions for each isotopologue.

- For a linear diatomic molecule [4]:

$$\nu = 2B_\nu(J+1) - 4D_\nu(J+1)^3 + E_Q + \cdots$$

| Input | Output |

- B (Rotational Constant)
- D (Centrifugal Distortion)
- eQq (Electric Quadrupole Hyperfine Constant)

SPCAT → Predictions of Hyperfine Transitions

- For quadrupole constant eQq, I relied on calculations of this parameter for each isotopologue by Petrov et al. in St. Petersburg, Russia [5].

- To calculate B and D, I performed weighted analyses of measurements of this parameter for ^{180}HfF$^+$ by JILA in 2012 [6].

- I then translated rotational parameters for ^{180}HfF$^+$ to ^{177}HfF$^+$ and ^{179}HfF$^+$ using isotopic scaling [7].

$$\frac{B_{177}}{B_{180}} = \left(\frac{\mu_{180}}{\mu_{177}} \right) \quad \text{and} \quad \frac{D_{177}}{D_{180}} = \left(\frac{\mu_{180}}{\mu_{177}} \right)^2$$

Calculated Parameters and Transitions:

Parameter	^{177}HfF$^+$	^{179}HfF$^+$
B (MHz)	9153.304	9143.372
D (kHz)	5.288	5.282

^{177}HfF$^+$			^{179}HfF$^+$		
Transition	Frequency (MHz)	Relative Intensity	Transition	Frequency (MHz)	Relative Intensity
F = 7/2 ← 7/2	18007.878	32	F = 9/2 ← 9/2	17968.116	33
F = 9/2 ← 7/2	18412.768	42	F = 11/2 ← 9/2	18408.110	40
F = 5/2 ← 7/2	18533.428	26	F = 7/2 ← 9/2	18508.704	27

Uncertainty of Predictions

A. Uncertainty of Isotopic Scaling Method

- HfO is isoelectronic to HfF$^+$ and has been studied with high-precision [8].

- To test method, I predicted known hyperfine transitions of ^{177}HfO & ^{179}HfO, using ^{180}HfO as anchor.

- Disagreement with observed frequency was $\lesssim$ **40 kHz**.

B. Uncertainty of eQq Calculation

- A $\pm 3\%$ variation in eQq value led to variations in the predictions of $\sim$ **10, 4,** & **7 MHz** respectively.

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