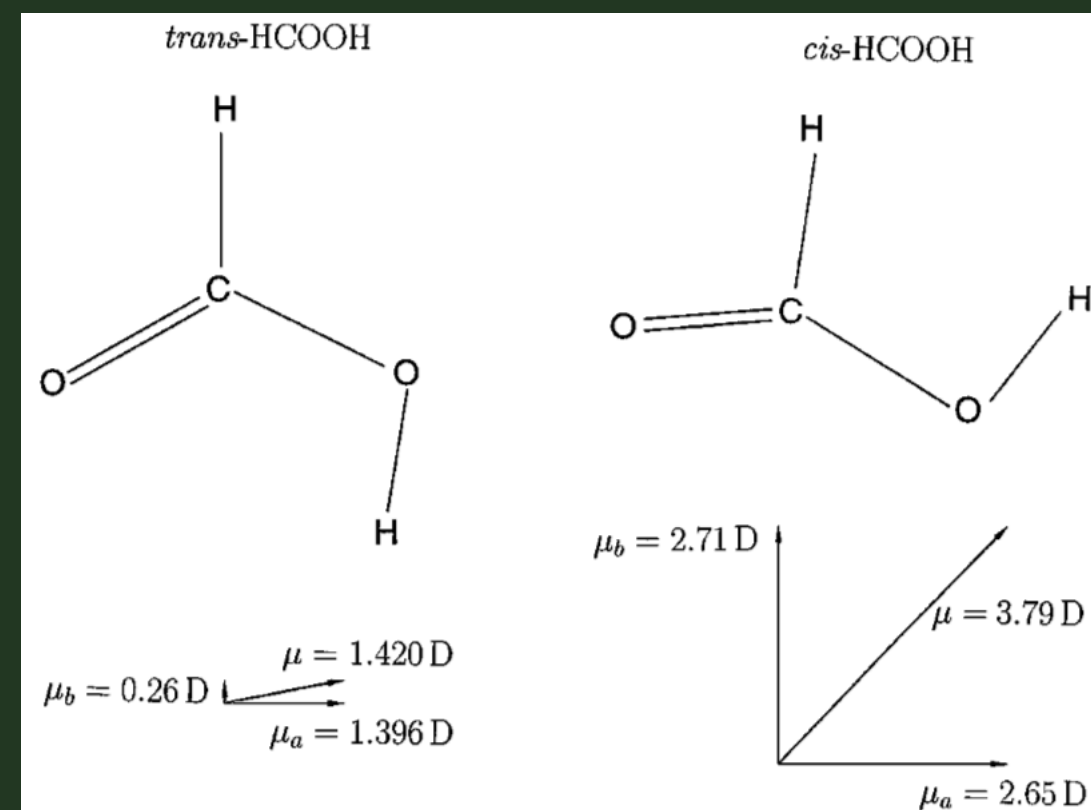


HIGH-RESOLUTION INFRARED SPECTROSCOPY OF A NON-NATIVE FORMIC ACID CONFORMER

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- There is a lack of experimental information compared to the “native” *trans* isomer
- *cis*-HCOOH has a greater dipole moment along the a- and b-axes relative to *trans*-HCOOH
- A good way to explore the HCOOH PES, and judge the *ab initio* predictions
- Possible astrophysical origin of HOCO



Winnewisser *et al.* JMS **216**, 259–265 (2002)

EXPT(SHIMANOUCHI, 1972)

*Perrin *et al.* 2002

CCSD(T)/ANO1

sym	#	vibration	v (cm ⁻¹)		v (cm ⁻¹)	IR (km/mol)	ω (cm ⁻¹)	IR (km/mol)
a	9	Torsion	640.72506(39)*		639.09	140	671.78	141
a	8	CH bend	1033		1034.55	2	1057.05	2
a'	7	OCO deform	626.16561(39)*		622.78	42	628.56	45
a'	6	C-O str	1105.3		1102.51	248	1133.19	250
a'	5	OH bend	1229		1215.40	4	1319.72	11
a'	4	CH bend	1287		1386.18	3	1411.18	3
a'	3	C=O str	1770		1781.64	294	1816.56	313
a'	2	CH str	2942.8		2931.07	26	3098.43	35
a'	1	OH str	3570		3574.34	52	3764.86	62

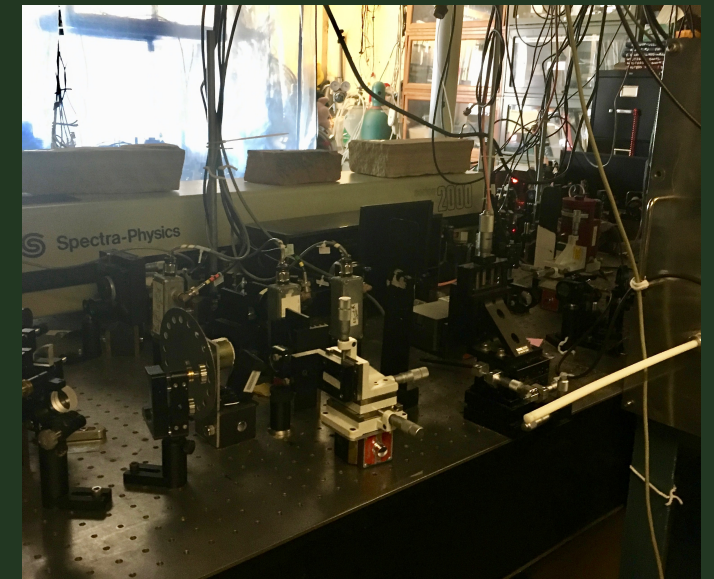
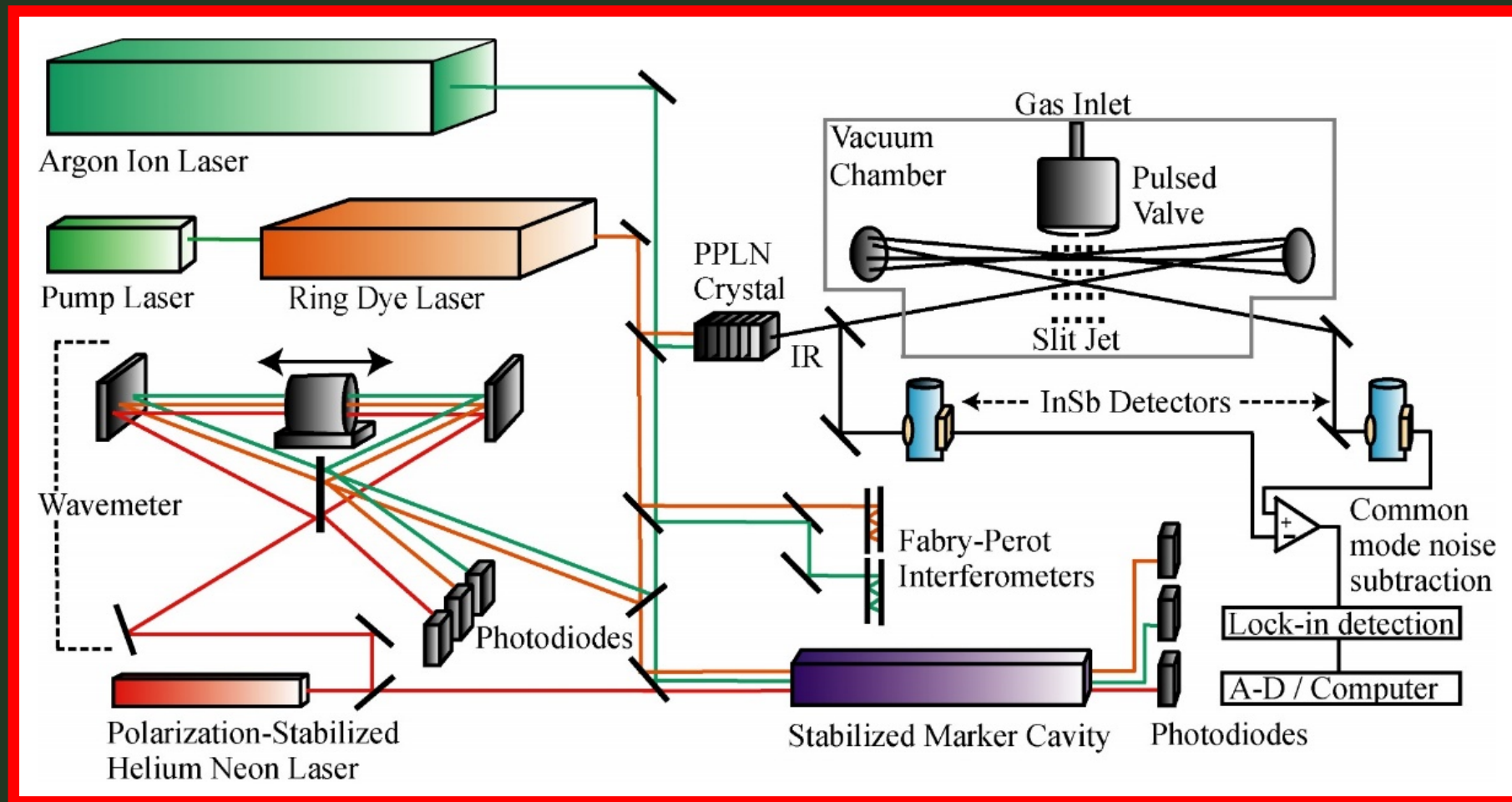
➔ Calculated using CFOUR

EXPT (MEYER, SUBMITTED)
*Baskakov *et al.* 2006

CCSD(T)/ANO1

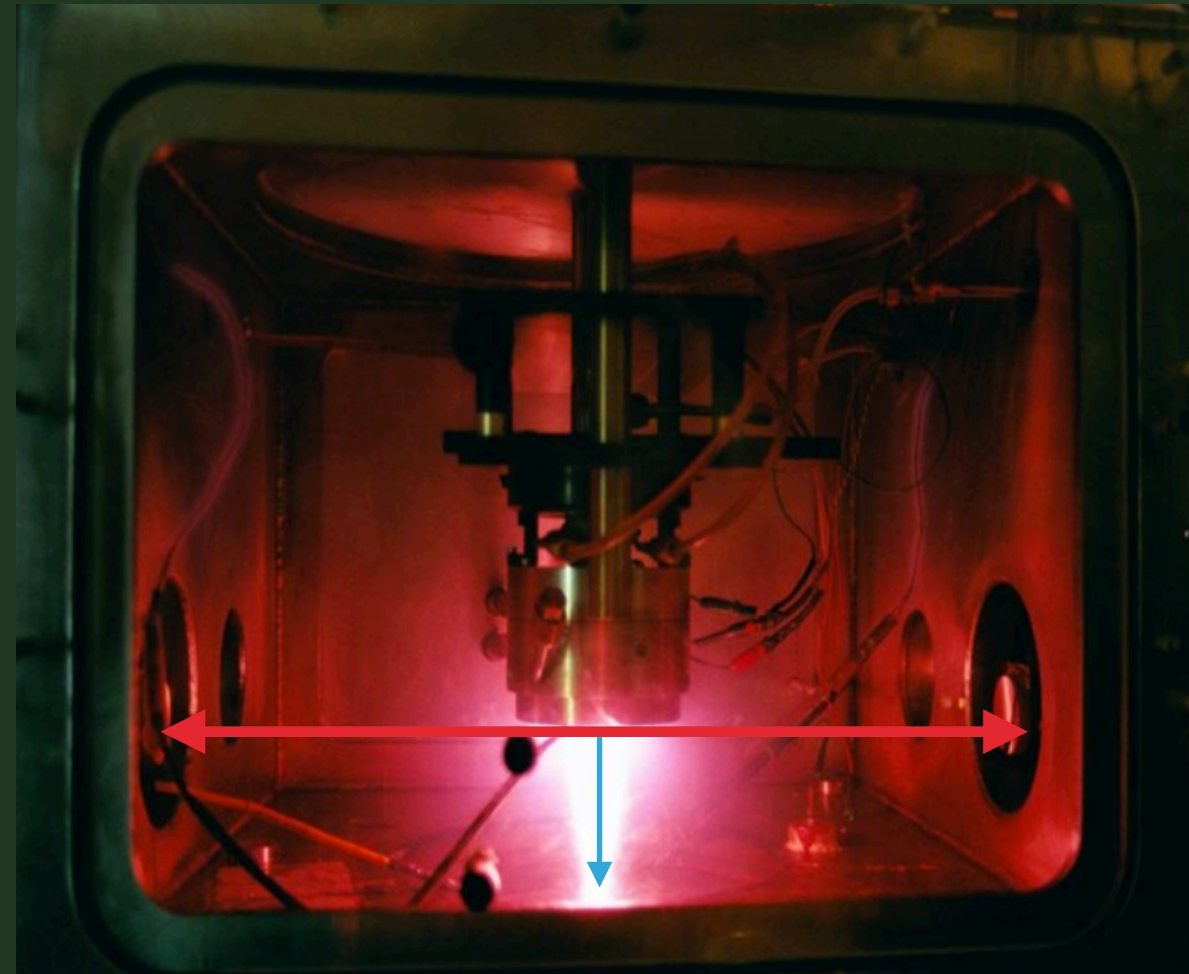
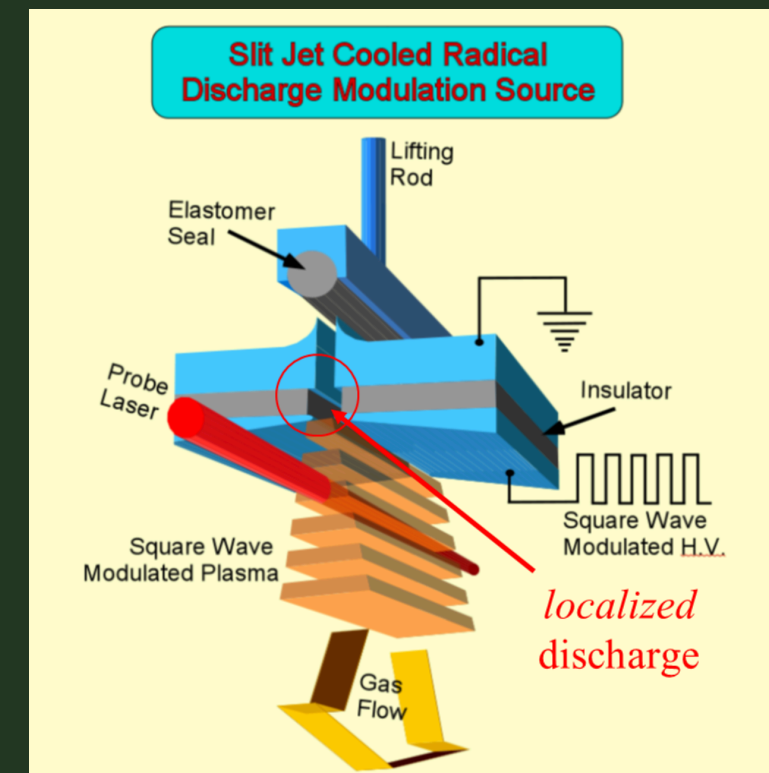
sym	#	vibration	v (cm ⁻¹)		v (cm ⁻¹)	IR (km/mol)	ω (cm ⁻¹)	IR (km/mol)
a	9	Torsion	493.420509(7)*		488.30	83	519.30	85
a	8	CH bend			1014.81	0	1035.81	0
a'	7	OCO deform			653.92	9	660.31	10
a'	6	C-O str	1093		1097.46	46	1120.68	48
a'	5	OH bend			1249.27	297	1291.05	305
a'	4	CH bend			1393.08	0.3	1427.60	0.2
a'	3	C=O str	1818		1822.07	233	1858.20	252
a'	2	CH str	2873		2869.55	64	3013.39	64
a'	1	OH str	3637		3640.31	51	3828.49	62

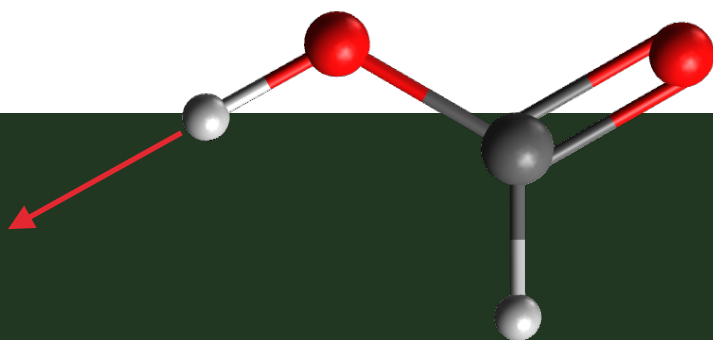
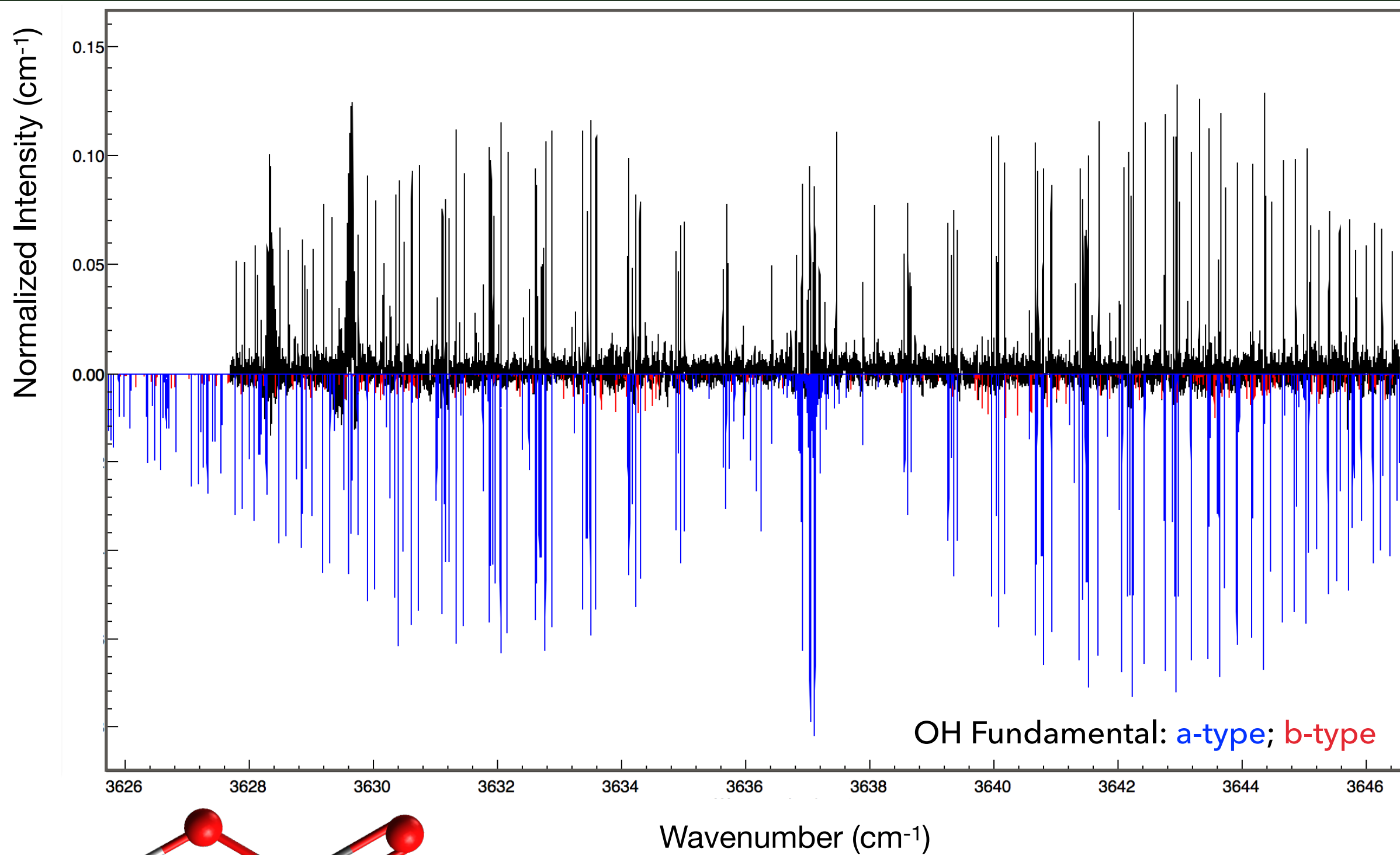
➔ Calculated using CFOUR

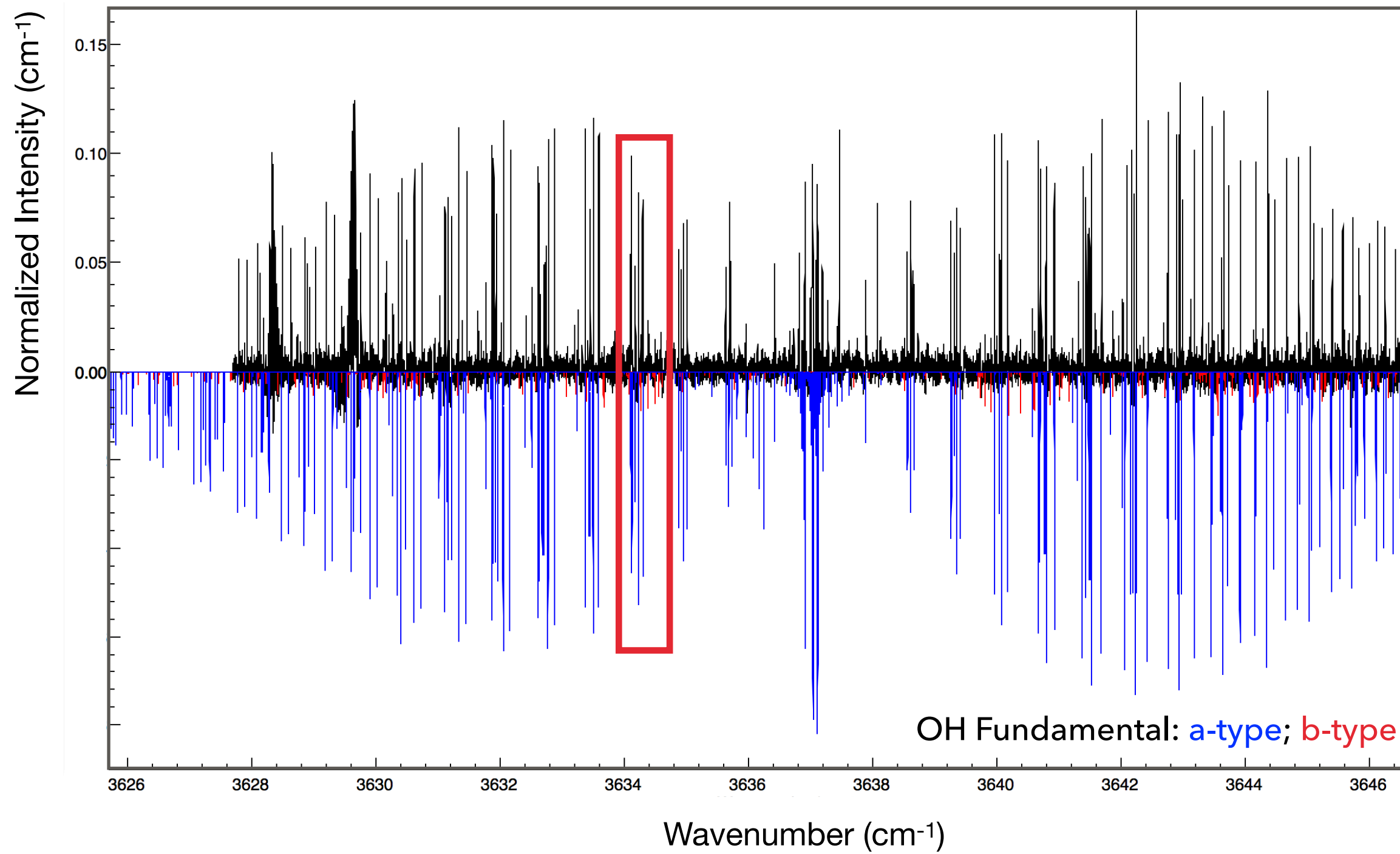


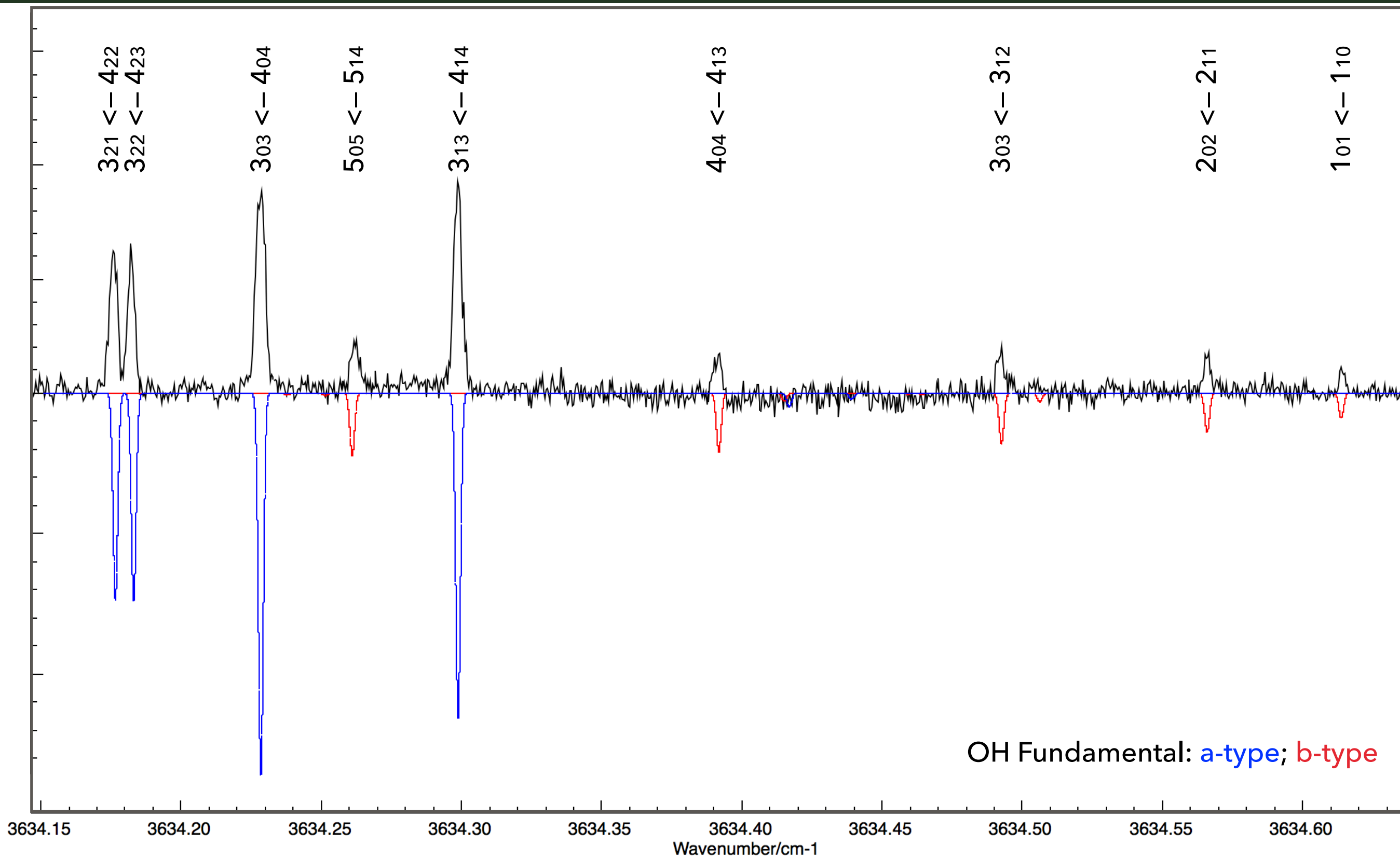
- ➔ Tunable 1 MHz resolution IR light
- ➔ Quantum shot noise limited absorbance sensitivity
- ➔ Suppressed Doppler absorption linewidths (≤ 60 MHz)

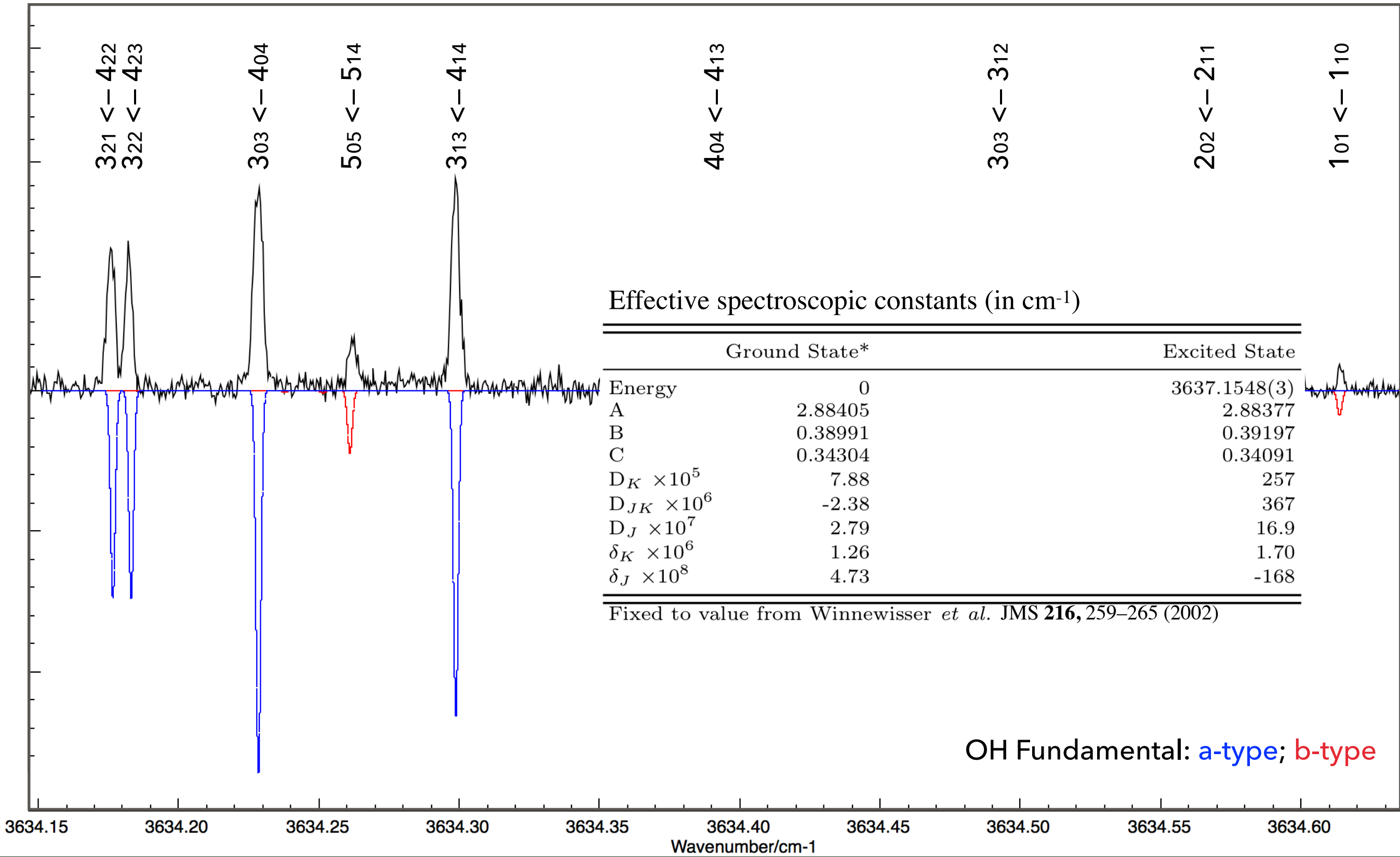
- Ar : Ar bubbled through HCOOH : H₂
- Supersonic planar plasma expansion
- Thin slit discharge nozzle (0.3x40mm)
- Applied HV = -650 V

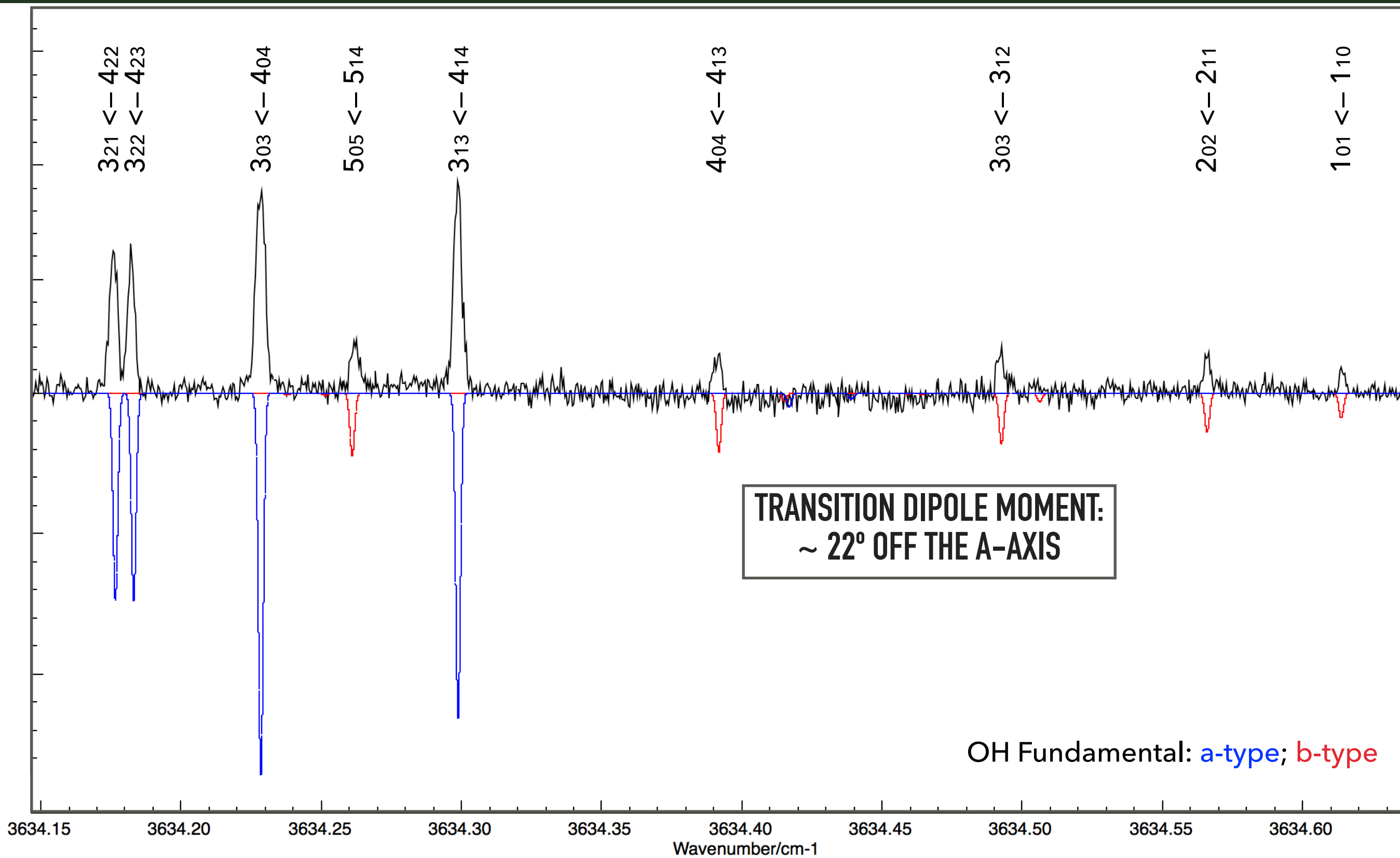












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- ➔ Rotationally resolved spectrum of the non-native isomer of HCOOH is measured between 3629 – 3650 cm^{-1}
 - ➔ The resulting data offers an additional method to search for this molecule in *e.g.* interstellar ices
 - ➔ The results are the start of a detailed study of the HCOOH PES
 - Future work includes the CH stretches around 2900 cm^{-1}

- ➔ Thanks to the Nesbitt Group
- ➔ Funding:
NSF, DOE, National Research Council (NRC) Fellowship

