The Millimeter-Wave Spectroscopy of Hydantoin, A Potential Precursor of Glycine

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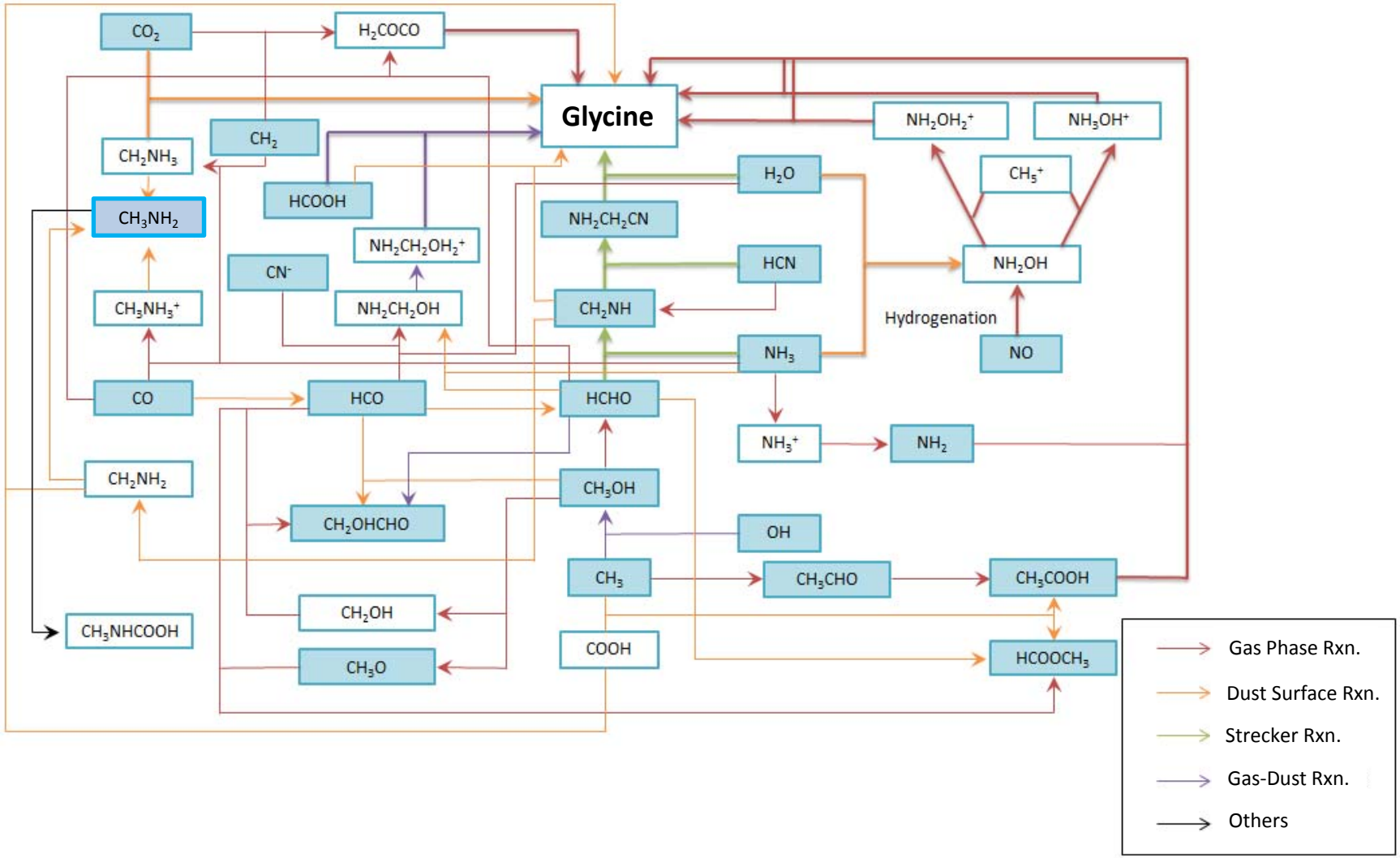
2016 Jun 21st

International Symposium on Molecular Spectroscopy, Illinois

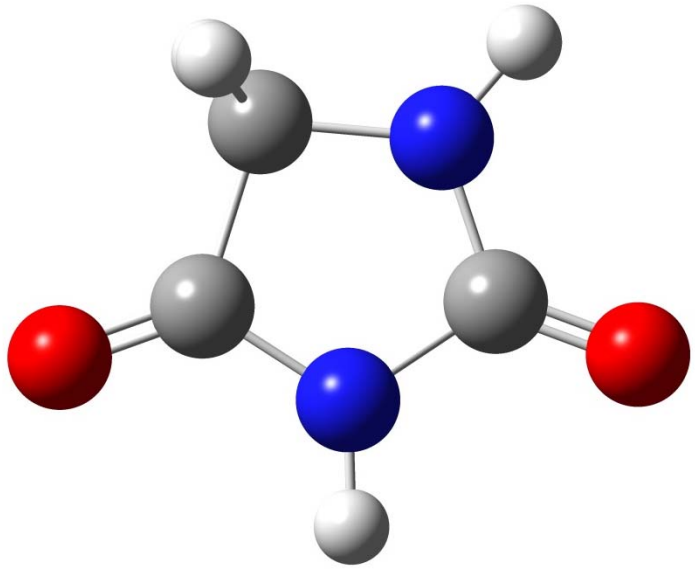
Road to Glycine



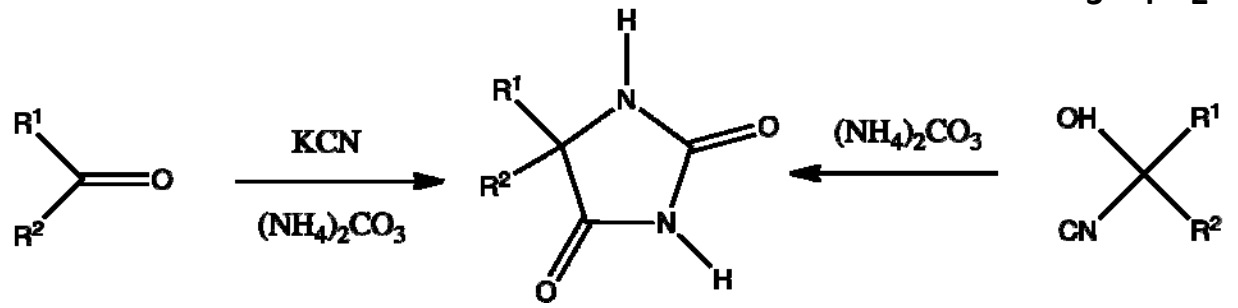
Hydantoin (Imidazolidine-2,4-dione)

- White powder (m.p. 220 ℃)

- Synthesized from glycolic acid and Urea
- Synthesized from Carbonyl compounds via Bucherer-Bergs Reaction
- Provides glycine by hydrolysis
- 5-substituted derivatives will lead to various kinds of amino acids



$C_3H_4N_2O_2$



5-substiuted Hydantoin

Aim of the study

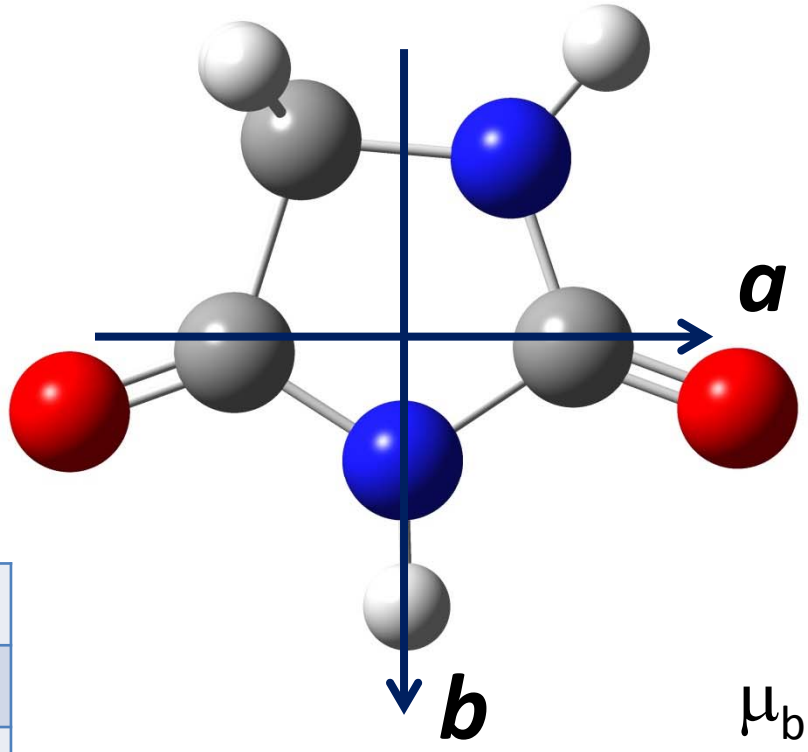
- To provide spectroscopic data for astronomical search

Previous spectroscopic studies on Hydantoin

- X-ray crystallography
  - Y. Fang-Lei et al. (2005)
- IR spectroscopy (solid) and ab initio
  - O. Gluce et al. (2012)
- Matrix isoleation IR spectroscopy and ab initio
  - G. O. Ildiz et al. (2013)
- Theoretical calculation
  - S. Belaidi et al. (2015)

- No gas phase data

Molecular structure & Dipole moment of Hydantoin



A	**~ 6500 MHz**
B	**~ 2300 MHz**
C	**~ 1700 MHz**

$\mu_b \sim 3.3$ D

Millimeter-wave spectroscopy of Hydantoin

- Conventional frequency modulated spectrometer with 100 cm length free space cell @ Toho university

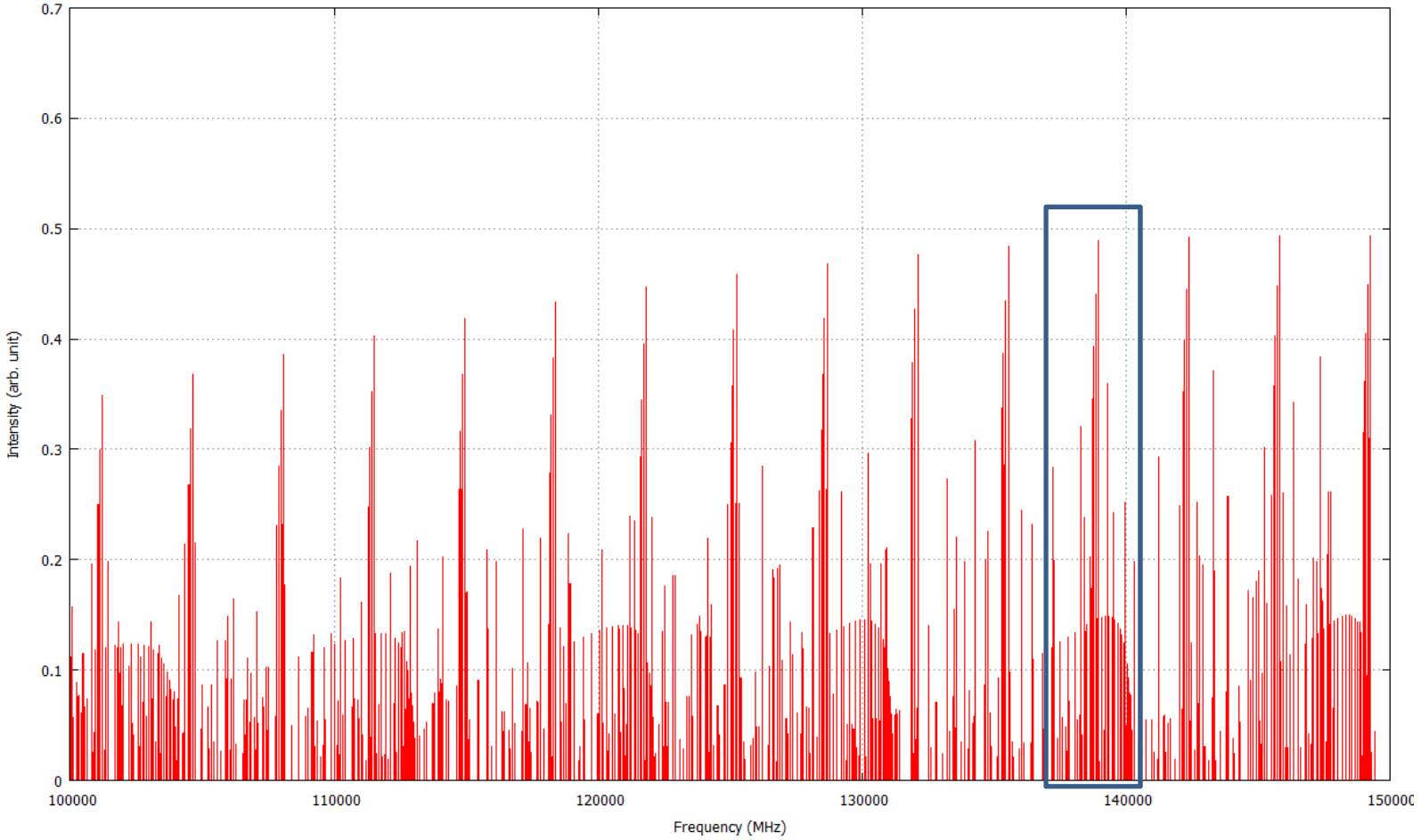
- Experimental Condition
  - Sample : Commercially available sample (20 g)
  - Heated to 420 K

    ➔ Hydantoin does not decompose at this temperature

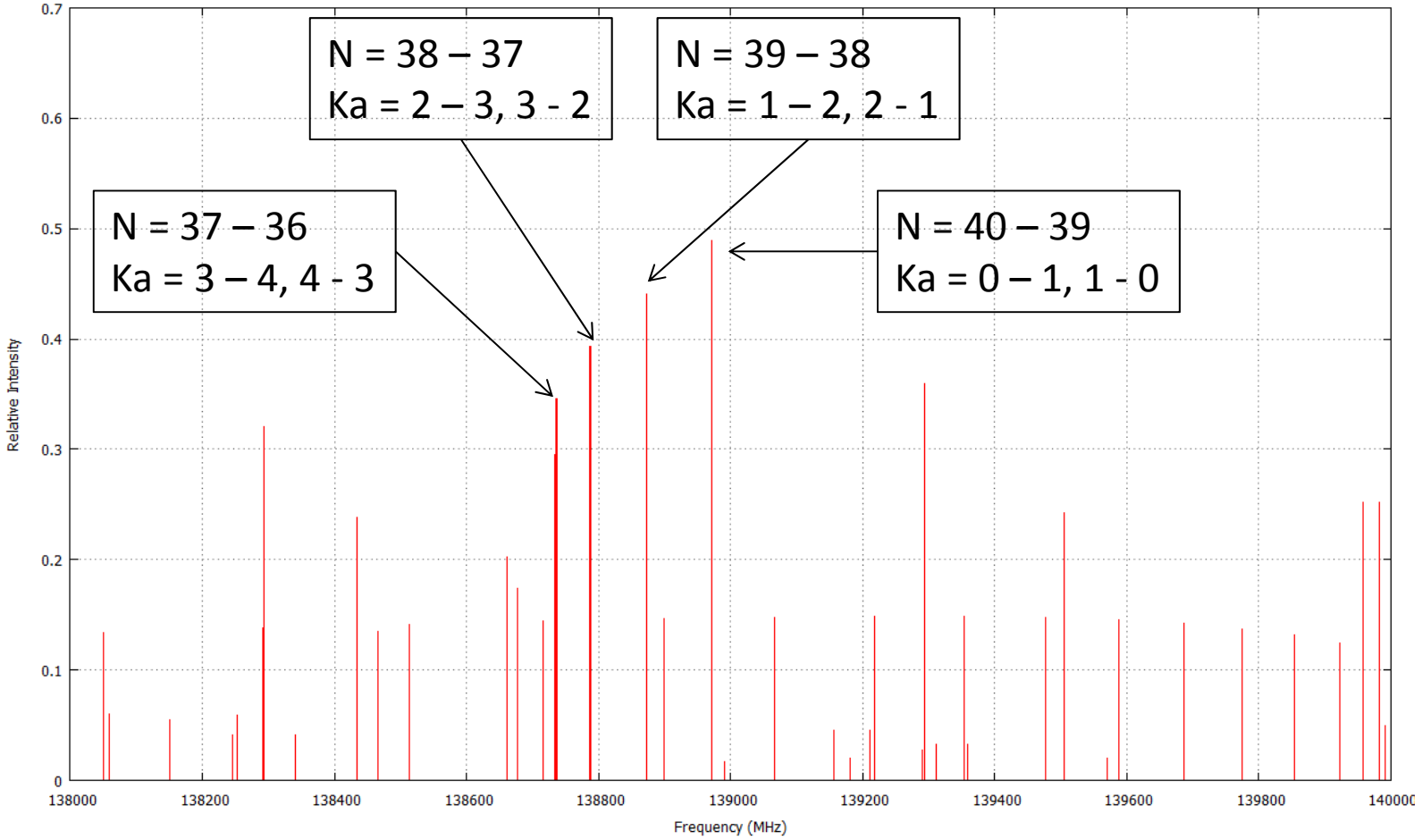
- Spectral measurement
  - Frequency region : 80 – 150 GHz
  - Search for b-type transitions

Predicted b-type spectrum

- Series with 3400 MHz separation @ ～140 GHz

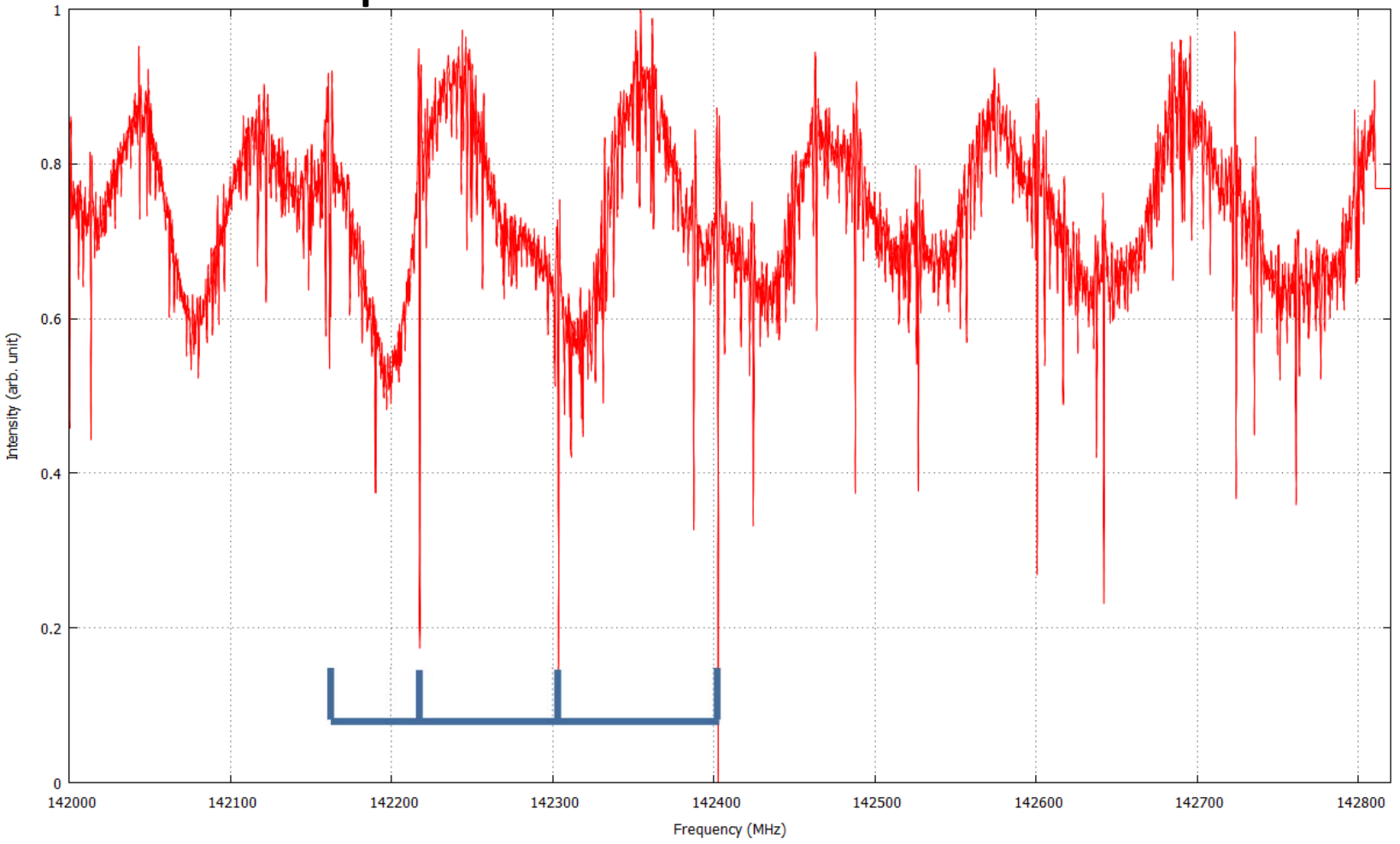


Predicted b-type spectrum



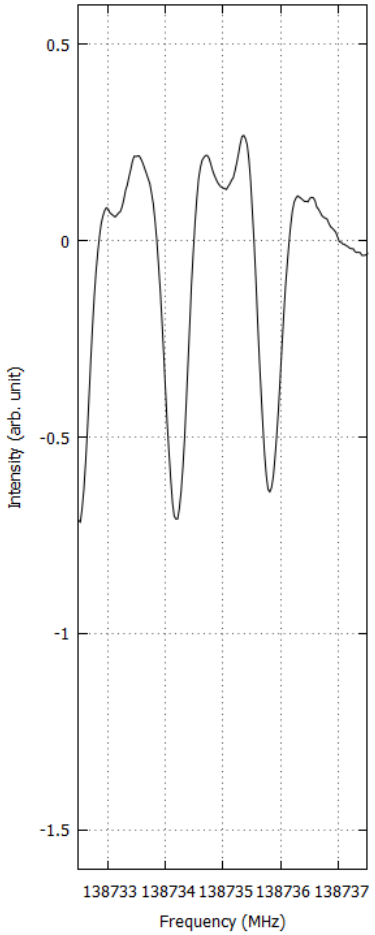
Spectral line survey @ 142 GHz

- 800 MHz span

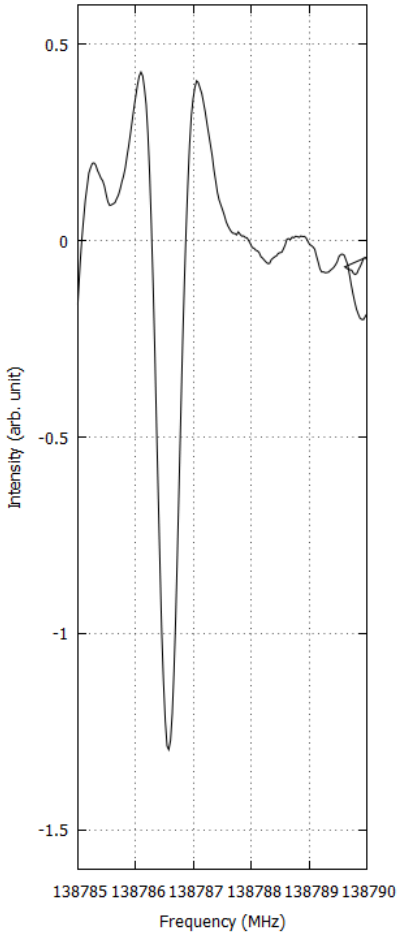


Spectral line survey @ 142 GHz

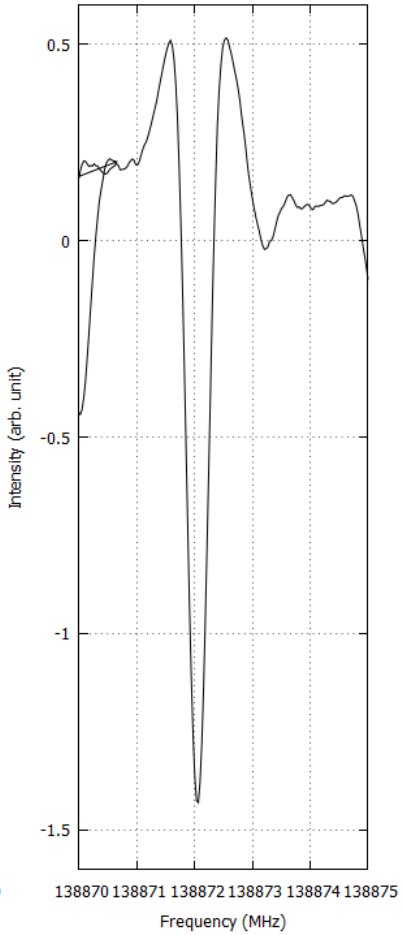
N = 37 – 36
Ka = 3 – 4, 4 - 3



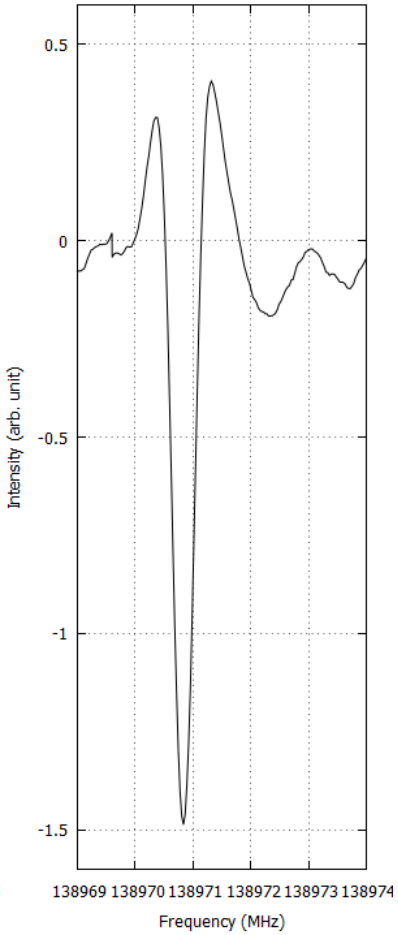
N = 38 – 37
Ka = 2 – 3, 3 - 2



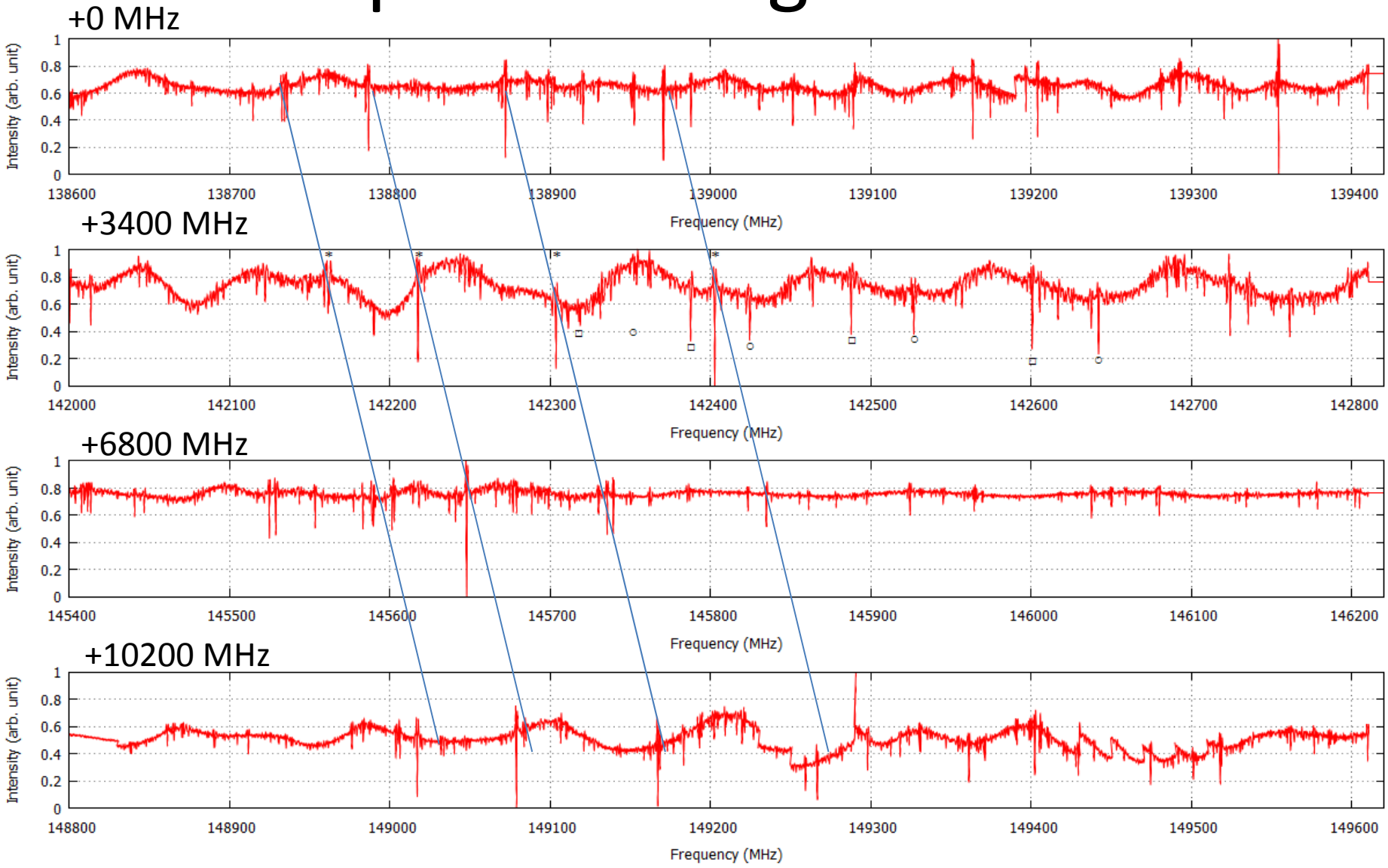
N = 39 – 38
Ka = 1 – 2, 2 - 1



N = 40 – 39
Ka = 0 – 1, 1 - 0

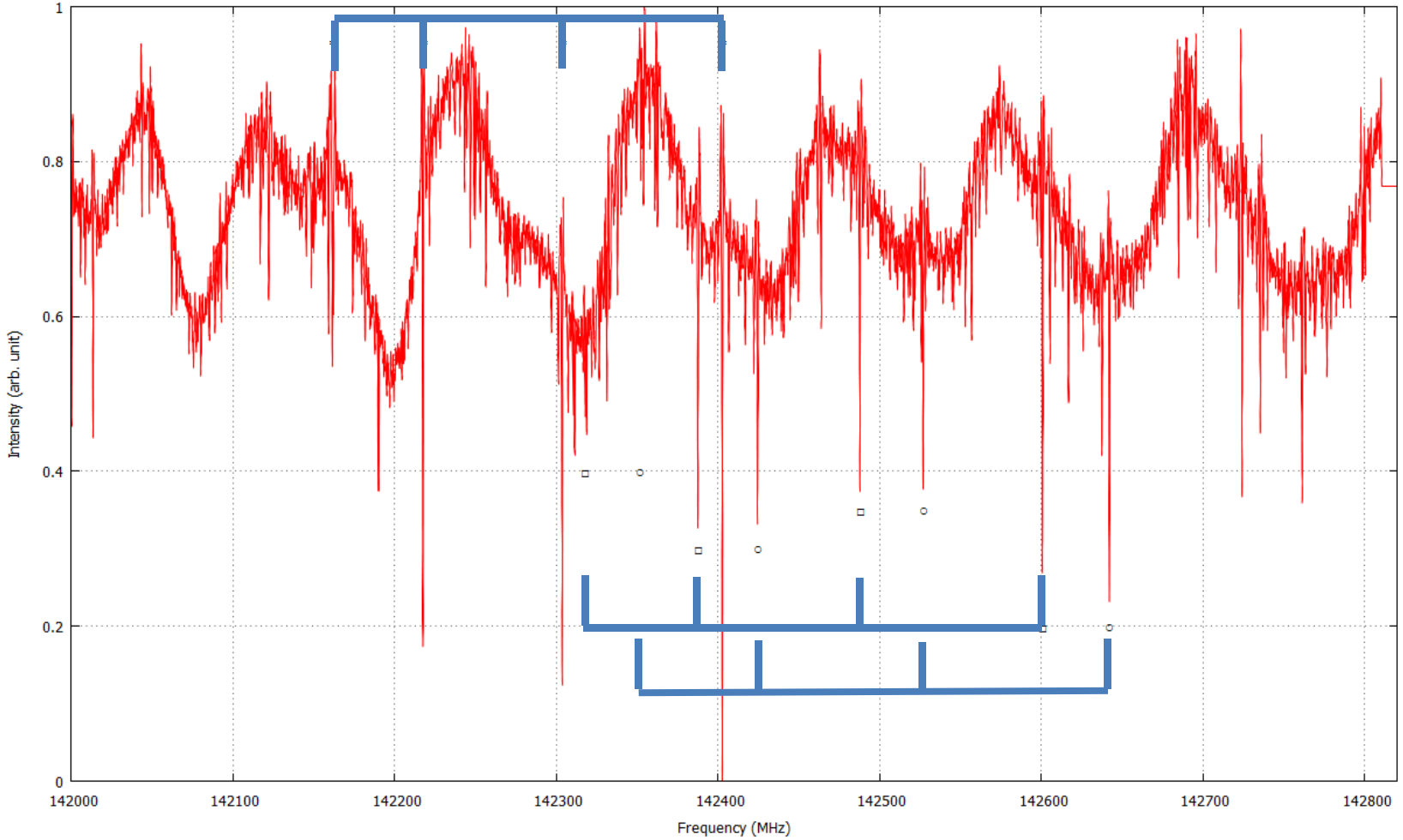


Spectral assignments

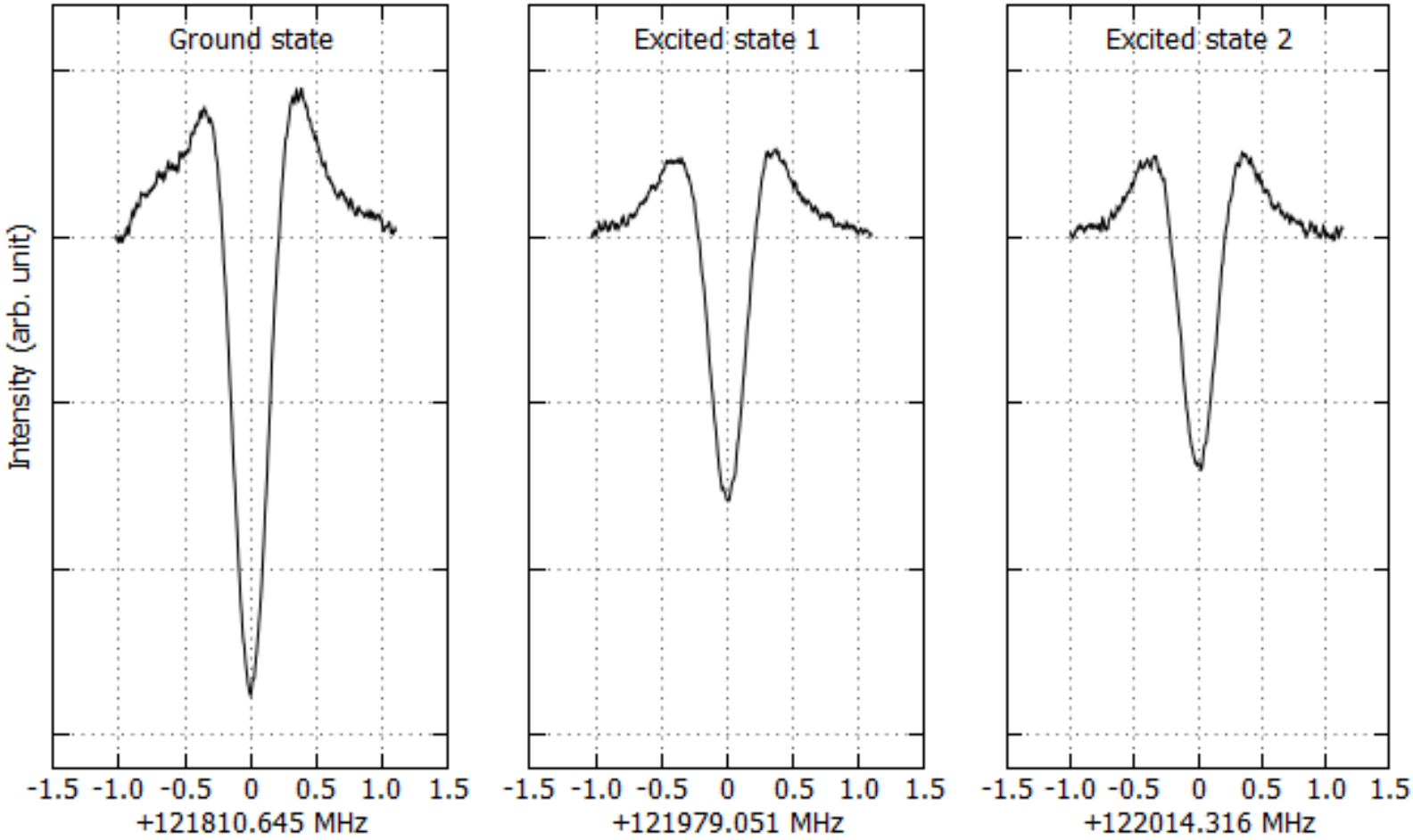


Spectral assignments

- b-type R-branch transition



Spectral Intensity @ 420 K
N = 35 - 34, Ka = 0-1,1-0 (121 GHz)



Intensity: Ground state > Excited state 1 > Excited state 2

Estimated vibrational energy

Present Study

	Relative Intensity	Estimated energy (cm^{-1})
Excited state 1	0.61	145
Excited state 2	0.55	175

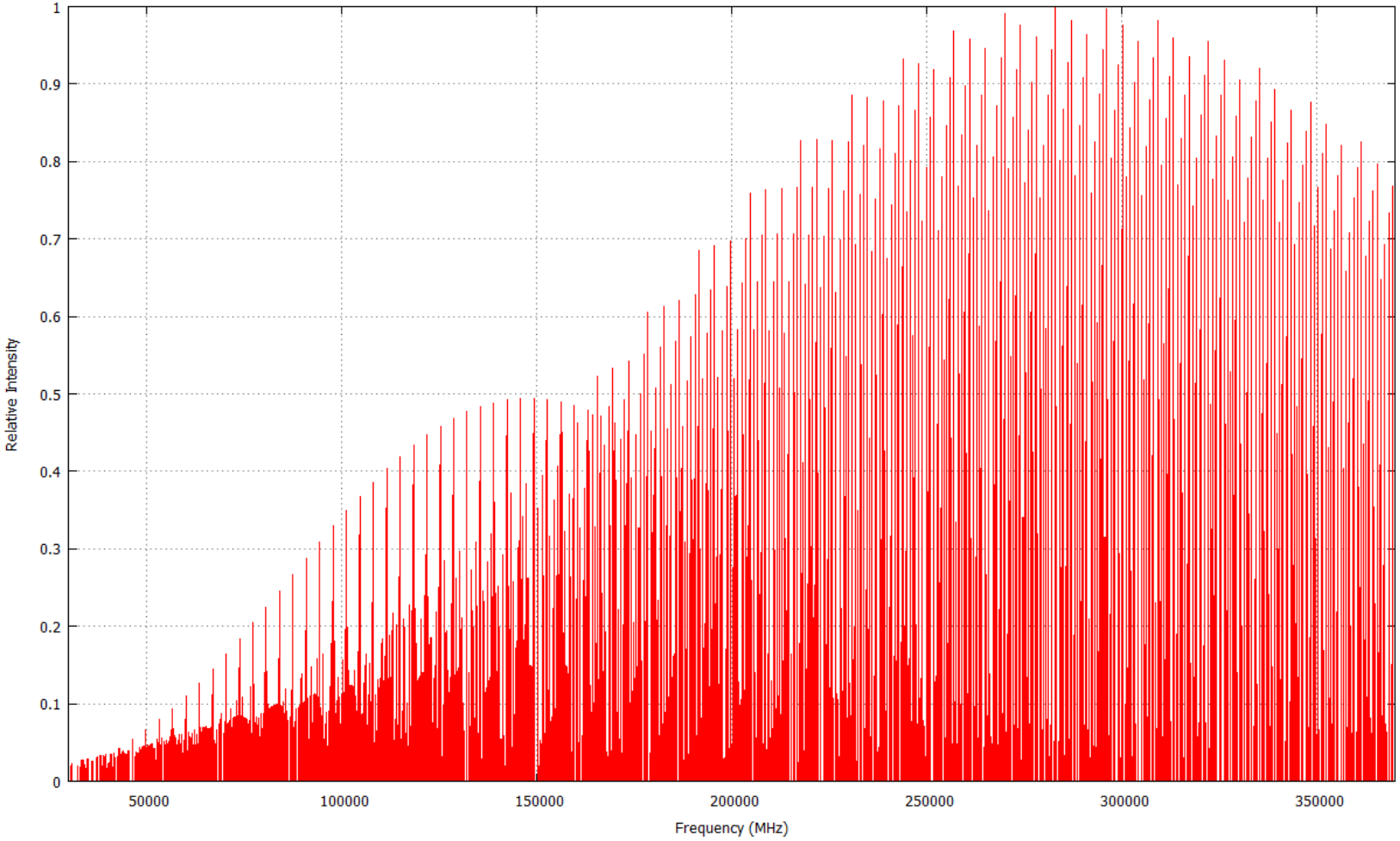
Comparison with calculations

Mode #	IR (Exp.)	DFT(B3LYP) 6-311G++(d,p)	DFT(B3LYP) 6-311G++(d,p)
	Ildiz et al.(2012)	Belaidi et al (2015)	Ildiz et al.(2013)
27		128.5824	29
26		144.7564	133
25		385.3754	356
24	428	389.9752	385

Excited state 1 → Mode 27 Excited state 2 → Mode 26

Hydantoin @ 100 K

- Ground state



Conclusions

- Pure rotational spectra of Hydantoin in the ground and 2 vibrationally excited states have been successfully assigned.

- Frequency catalogues are now ready for astronomical observation of Hydantoin below 300 GHz.

Acknowledgements

This work has been supported by JSPS Kakenhi (Grants-in-Aid for Scientific Research) #15H03646

Thank you for your attention.