Rotational spectroscopy of Pyrrole - A model for astronomical searches

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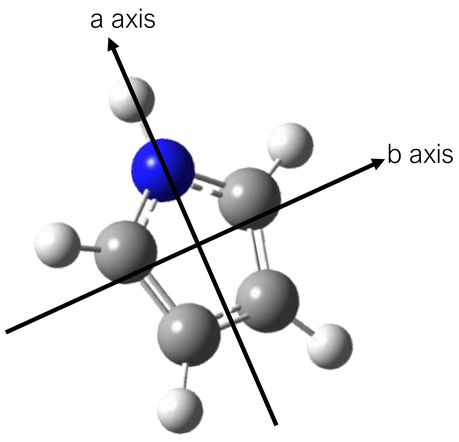
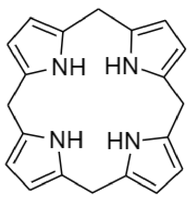
Pyrrole (*c*-C_4H_5NH)
- Planar molecule
- C_{2V} point group symmetry
- μ_a = 1.74(2) D, (L. Nygaard 1969)
- Melting point = 250 K
- Boiling point = 402-404 K

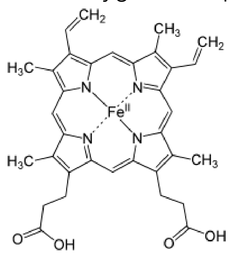


Applications of pyrrole
Pyrrole has been researched since 1952.
Tetrapyrroles – a four-unit structure of pyrrole.
Pyrrole and its derivatives are present antimicrobial, antiviral and anti-inflammatory drugs.

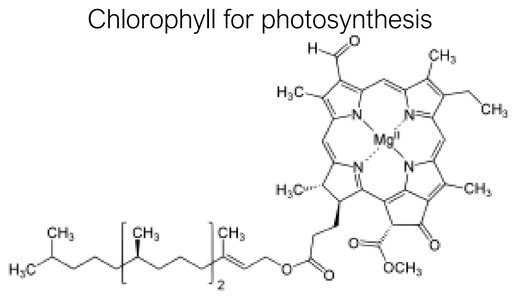
Porphyrin



Heme-B for oxygen transportation



Chlorophyll for photosynthesis



Global fitting and predictions- A unique global fitting was created by a combination of previous and our works on pyrrole.

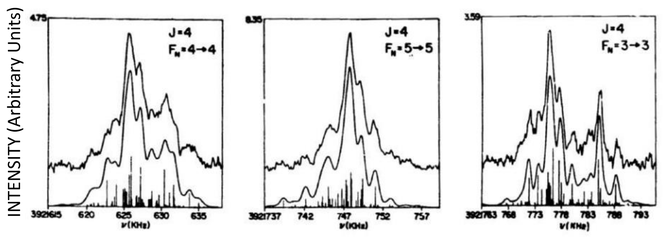
Parent species (v=0→0)
13-25 GHz (L.Nygaard 1969)
4-14 GHz (K.Bolton 1974) ^{13}C
1-5 GHz (S.R Hartmann and W.Happer 1974)
149-260 GHz (Wlodarczak 1988)
60-78 GHz NEW

(v=0 →1)
(D.W Tokaryk J.A van Wijngaarden 2009)

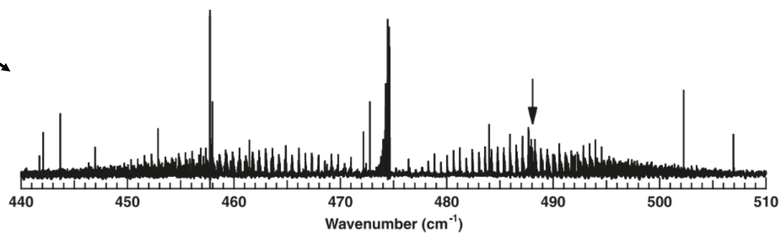
(v=1 →1)
NEW

Isotopologues
^{13}C ,^{15}N, D (L.Nygaard 1969)
^{13}C 60-78 GHz NEW

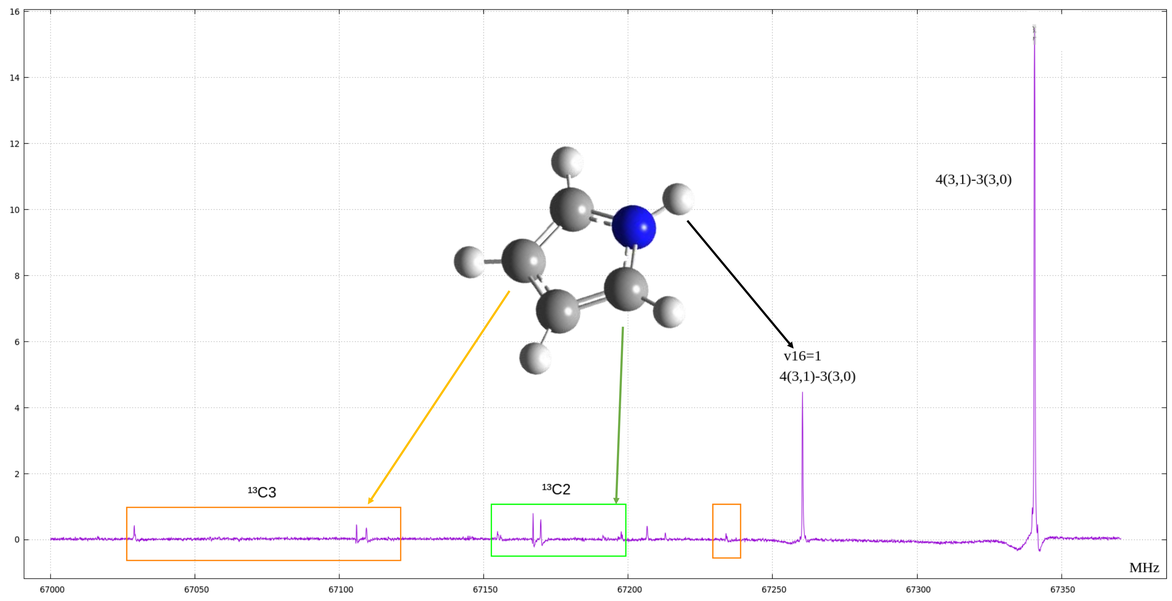
High resolution



IR



Rotational spectroscopy can distinguish between parent species, isotopologues and conformers. Also obtained new transition lines for the isotopologues and the vibration-rotation first excited state.

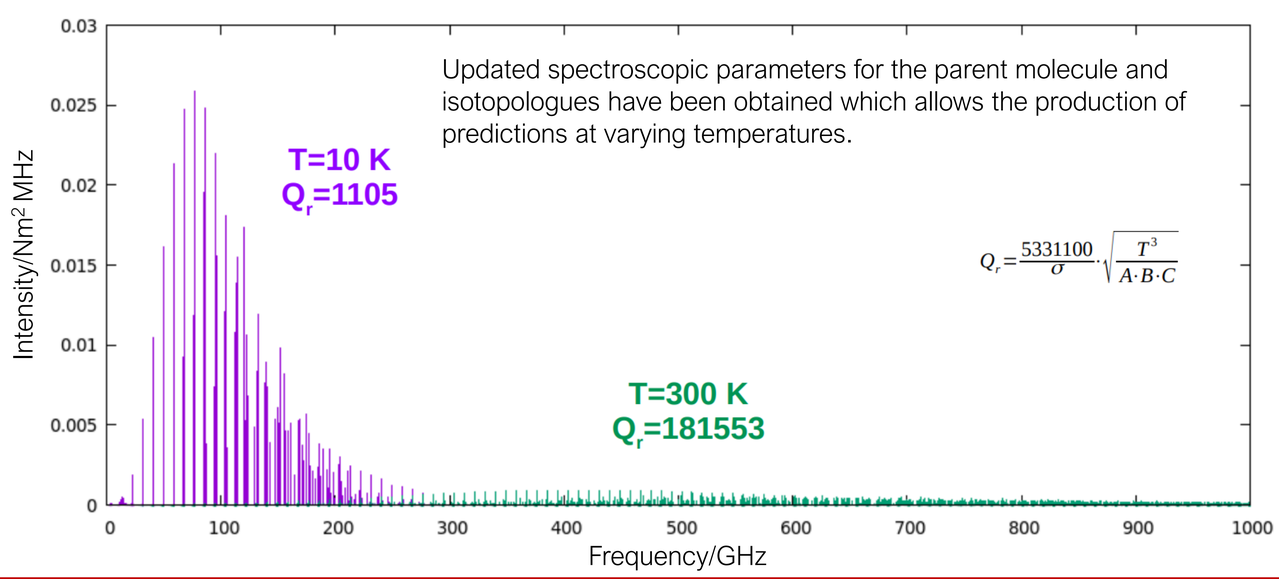


Free Jet Absorption Millimetre Wave (FJ-AMMW) Spectrometer – Rotational spectroscopy the unique pattern of each molecule allowing identification of species.
Instrument range = 60-78 GHz, resolution 0.3 MHz. From this, 28 new transition lines were measured.

Transition /J(Ka,Kc)'-J(Ka,Kc)''	Nuclear quadrupole coupling components / MHz			
4(3,1)-3(3,0)	67339.92	67340.69	67341.75	
3(2,1)-2(0,2)	67612.87	67613.73	67614.40	67615.10
5(3,3)-4(3,2)	67971.33	67971.65		
7(0/1,7)-6(0/1,6)	67982.46			
6(1/2,5)-5(1/2,4)	67985.08	67985.28		
8(1/2,7)-8(1/0,8)	67998.23			
5(4,2)-4(4,1)	76412.02	76412.28		
8(0/1,8)-7(0/1,7)	77046.44			
7(1/2,6)-6(1/2,5)	77049.00			
6(3,4)-5(3,3)	77052.22	77052.48		
6(2,4)-5(2,3)	77053.21	77053.49		
9(1/2,8)-9(1/0,9)	77064.61	77065.19		
4(4,0)-3(2,1)	77488.34	77488.61		
5(3,2)-4(3,1)	77608.26	77608.44	77609.16	

Molecular species	A / MHz	B / MHz	C / MHz
Parent	9130.6348(6)	9001.3641(5)	4532.1079(5)
v=1	9110.348(3)	8988.316(3)	4531.543(1)
^{15}N	9131.28(7)	8807.45(7)	4482.65(7)
$^{13}C_2$	9021.880(5)	8892.732(5)	4477.740(7)
$^{13}C_3$	9099.126(6)	8803.136(6)	4473.675(7)

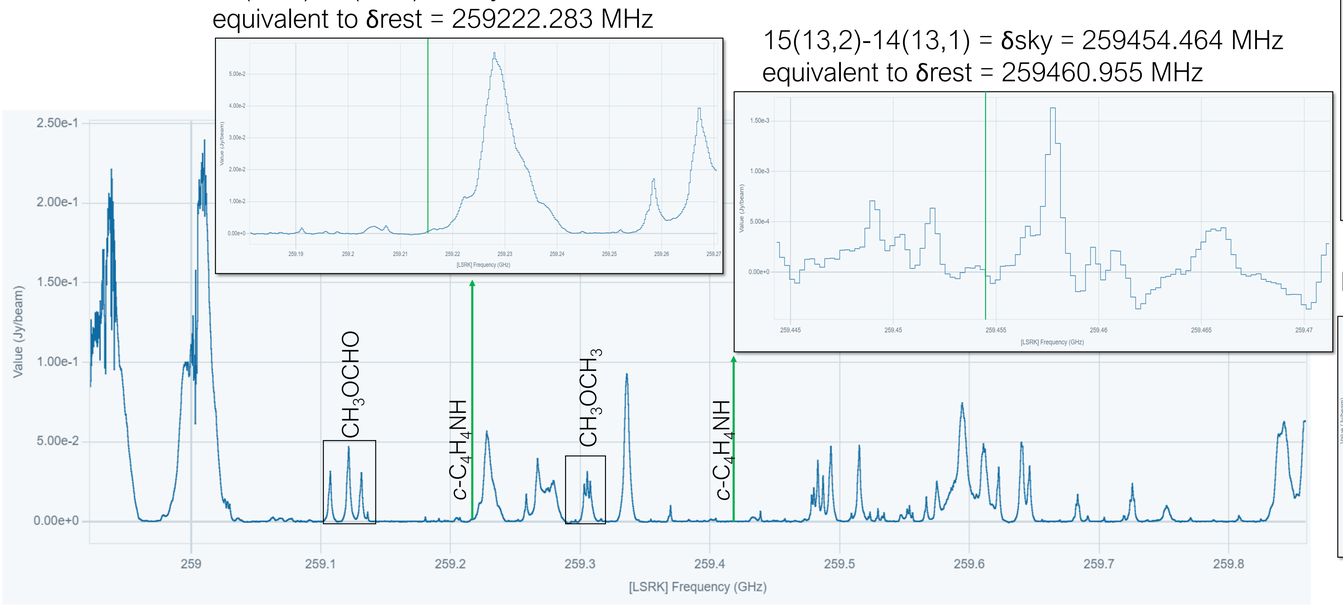
	D_J / kHz	D_{JK} / kHz	D_K / kHz	d_1 / kHz	d_2 / kHz
Parent	2.9283(6)	-4.653(1)	2.021(1)	0.0614(3)	0.0225(2)



Astronomical application - Aim to use the predicted rotational spectrum within the ALMA Archive database to search for pyrrole within astronomical surveys.
Over 200 molecular species have been detected in Interstellar medium via their rotational spectrum. (C.Cabezas 2020)
M42 Orion nebula - 2019.1.00246.S, (5^h:35^m:14.16^s, -5°:22′:21.5″), Δv_{LSR} = 7.5 km/s
Survey frequencies: δsky = 258922– 259859 MHz

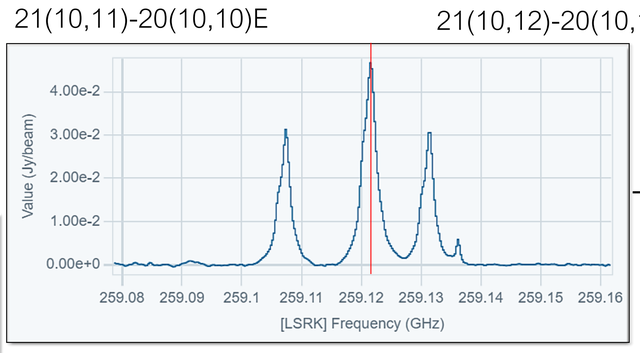
ΔK_a= 2
13(12,2)-12(10,3) = δsky = 259215.798 MHz
equivalent to δrest = 259222.283 MHz

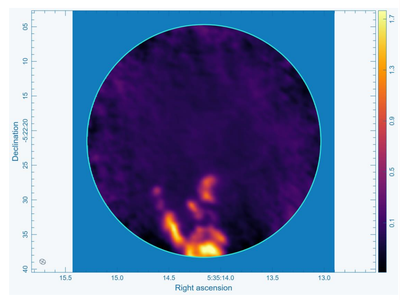
15(13,2)-14(13,1) = δsky = 259454.464 MHz
equivalent to δrest = 259460.955 MHz



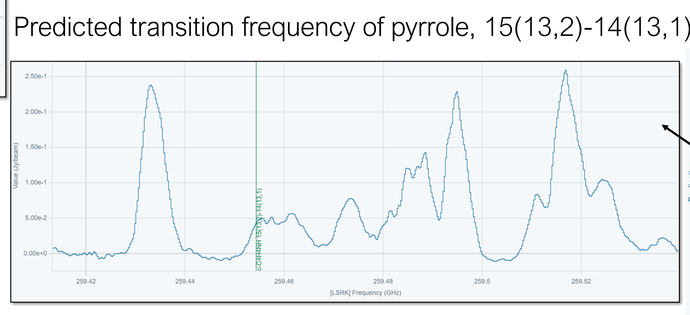
Methyl formate, CH_3OCHO - Δv_{LSR} = 7.5 km/s was determined due to the Methyl formate assignment.

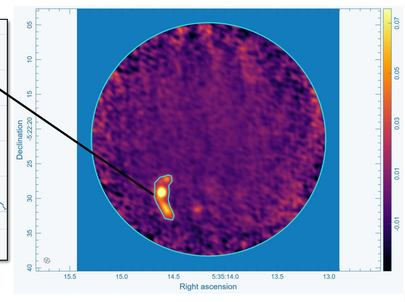
21(10,12/11)-20(10,11/10)A
21(10,11)-20(10,10)E
21(10,12)-20(10,11)E





Predicted transition frequency of pyrrole, 15(13,2)-14(13,1).





References- K.Bolton and R.D Brown, Australian Journal of Physics, 27, 1974, 143-146. C.Cabezas et al, Astronomy & Astrophysics, 636, 2020, A33. S.R Hartmann and W.Happer, Engineering, No. CU-6-74-0383.1974. L. Nygaard et al, Molecular spectroscopy, 3(6), 1969, 491-506. D.W Tokaryk J.A van Wijngaarden, Canadian Journal of Physics 87.5, 2009, 443-448. G. Wlodarczak et al, Journal of molecular spectroscopy, 127, 1988, 200-208.