

Free-jet Rotational Spectra of Urea Analogues: Laboratory Data for Future ALMA Band 2 Searches



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Key results

Measurements and assignments of the rotational spectrum of N-methylurea under supersonic expansion in the 8–18 GHz and 59.6–78.3 GHz ranges.

Modelling methyl internal rotation and ^{14}N nuclear quadrupole coupling splittings.

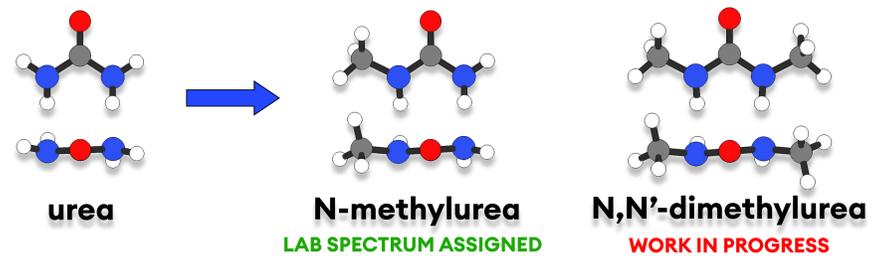
Providing a Band 2-ready spectral prediction for searches in astronomical surveys.

Urea and derivatives in space

The detection of urea in the ISM ($2.7 \times 10^{16} \text{ cm}^{-2}$ toward Sgr B2(N1), $6.3 \times 10^{12} \text{ cm}^{-2}$ toward G+0.693–0.027) raises the question of whether larger urea analogues could also be present.

^(a)A. Belloche, *A&A*, 628 A10 (2019)

^(b)I. Jiménez-Serra, *Astrobiology* 20, 1048–1066 (2020)

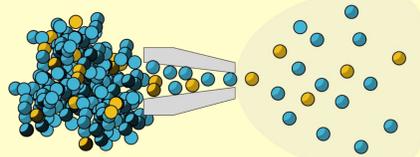


Free-jet absorption millimeter wave rotational spectrometer



Use of Free-jet Expansion

● COM ● He/Ne/Ar



$T \equiv T_{\text{rot}} = 298\text{--}400 \text{ K}$
 $P = 150\text{--}300 \text{ mbar}$

$T_{\text{rot}} \approx 10 \text{ K}$
 $P < 10^{-4} \text{ mbar}$

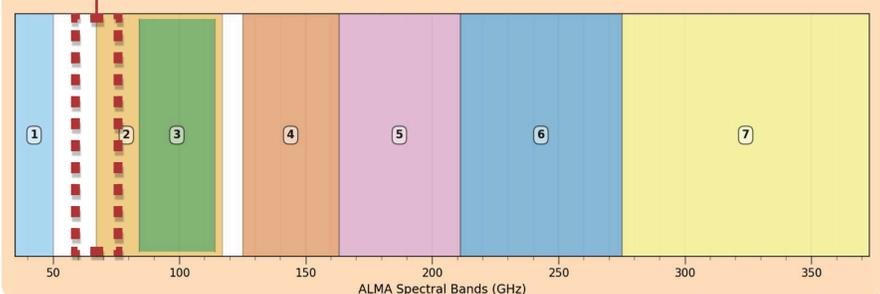
Cooling of vibrational and rotational levels enabling high-resolution rotational spectroscopy of complex organic molecules (COMs).

Overlap with ALMA Band 2 Frequency Region

Free-jet Frequency Range: 59.6–78.3 GHz

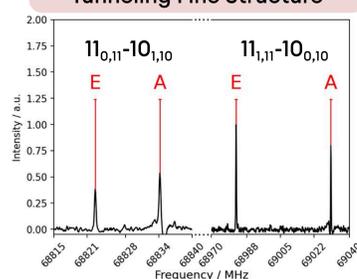
Resolution: 300 kHz Error: 50 kHz

Precise experimental reference data

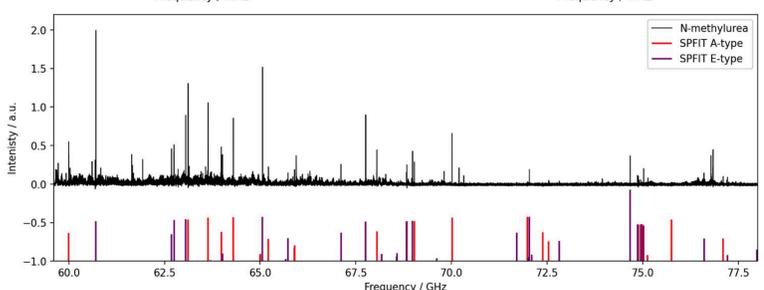
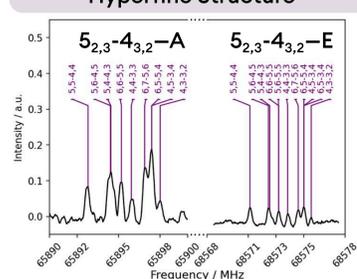


N-Methylurea: a complex rotational pattern

Methyl Internal Rotation Tunneling Fine Structure

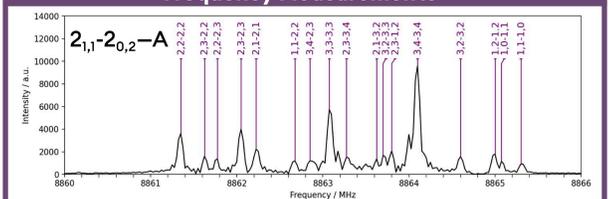


Nuclear Quadrupole Coupling Hyperfine Structure



Parameter	A-State	E-State
A / MHz	10666.801(2)	10451.270(4)
B / MHz	4079.5718(7)	4072.599(1)
C / MHz	3002.1902(7)	3003.0686(9)
N. lines	273	390
σ / kHz		22
N. param.		28
μ_a -type	N	N
μ_b -type	Y	Y
μ_c -type	Y	Y
$M_{aa} / \text{u}\text{\AA}^2$	122.41924(2)	122.012(3)
$M_{bb} / \text{u}\text{\AA}^2$	45.91753(2)	46.275(3)
$M_{cc} / \text{u}\text{\AA}^2$	1.46116(2)	2.080(3)

Determination of Nitrogen NQC Constants from Low Frequency Measurements

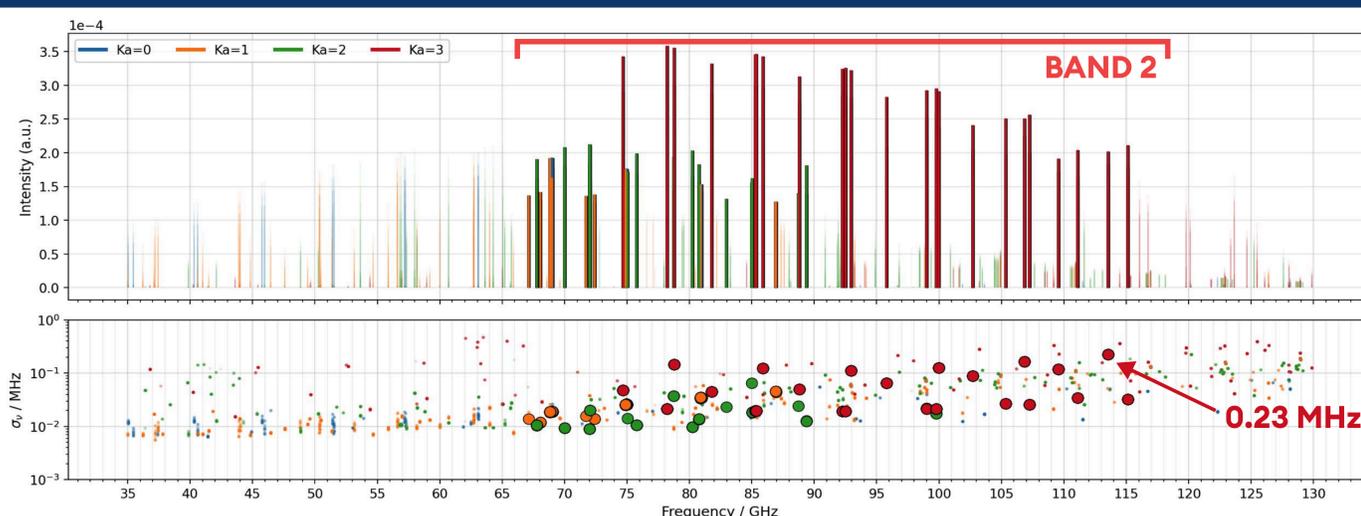


CP-FTMW Measurements from Dr. Nick Walker, Newcastle University

Determination of Methyl Internal Rotation Parameters

Parameter	MP2/aug-cc-pVTZ	Experimental
$\angle ia / ^\circ$	27.5695	27.3
$\angle ib / ^\circ$	63.0996	63.7
$\angle ic / ^\circ$	95.5943	90.0
$I_a / \text{u}\text{\AA}^2$	3.152	3.152
V_3 / cm^{-1}	244	113
$\Delta_0 / \text{cm}^{-1}$	0.11	1.03

Predicted absorption spectrum for N-methylurea (T=10 K)



Predicted rotational transitions highlighting in bold the top high-intensity lines with low frequency uncertainty as candidate target for astronomical surveys.

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Dr. Charlotte N. Cummings, and Dr. Nick Walker of Newcastle University for recording the CP-FTMW experimental spectra