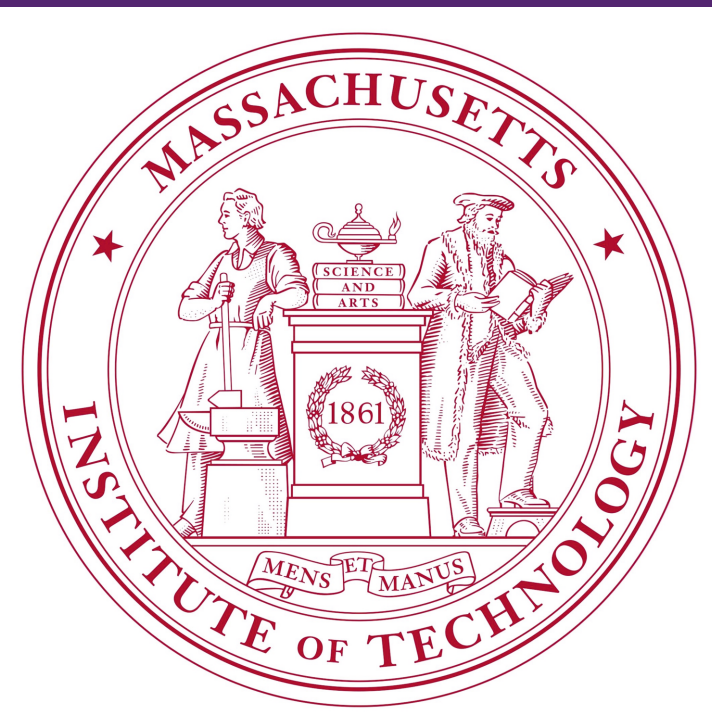




Fourier-transform spectroscopy and deperturbation analysis of the $A^1\Pi$ ($v = 0$) level in the $^{12}\text{C}^{17}\text{O}$ isotopologue



R. Hakalla^a, W. Szajna^a, A. N. Heays^{b,c,d}, N. de Oliveira^e, E. J. Salumbides^b, M. Ostrowska-Kopeć^a, I. Piotrowska^a, P. Kolek^a, M. Zachwieja^a, R. Kępa^a, R. W. Field^f, and W. Ubachs^b



^aMaterials Spectroscopy Laboratory, Faculty of Mathematics and Natural Science, University of Rzeszów, Poland
^bDepartment of Physics and Astronomy, and LaserLab, Vrije Universiteit, Amsterdam, The Netherlands
^cLERMA, Observatoire de Paris, CNRS, Sorbonne Universités, UPMC Univ. Paris 06, Meudon, France
^dSchool of Earth and Space Exploration, Arizona State University, Tempe, AZ 85281, USA
^eSynchrotron SOLEIL, Orme de Merisiers, St. Aubin, Gif sur Yvette Cedex, France
^fDepartment of Chemistry, Massachusetts Institute of Technology, Cambridge, USA



Summary

The present study focuses on a first analysis of spectroscopic data of the $A^1\Pi$ ($v = 0$) level in $^{12}\text{C}^{17}\text{O}$. VIS-FT spectroscopy (1.71 m Bruker IFS 125-HR) was used to obtain the $B^1\Sigma^+ - A^1\Pi$ (0, 0) band spectrum under 0.018 cm^{-1} resolution.

The discharge was conducted in the air-cooled, carbon hollow-cathode lamp. Then $^{17}\text{O}_2$ (70%) with $^{16}\text{O}_2$ (30%) was admitted. The temperature of dc-plasma at the center of the cathode was ~ 1000 K. The fitting uncertainty of the line frequency measurements was estimated to be 0.005 cm^{-1} .

The spectrum was combined with high-resolution photoabsorption measurements of the $^{12}\text{C}^{17}\text{O}$ $B^1\Sigma^+ - X^1\Sigma^+$ (0, 0) and $C^1\Sigma^+ - X^1\Sigma^+$ (0, 0) bands recorded with an accuracy of 0.01 cm^{-1} using the VUV-FT spectrometer installed on the DESIRS beamline at the SOLEIL synchrotron.

An effective Hamiltonian used in deperturbation analysis was performed up to $J = 39$, quantitatively addressing complex, multistate interactions with the $e^3\Sigma^-$ ($v = 1$), $d^3\Delta$ ($v = 4$), $a^3\Sigma^+$ ($v = 9$), $D^1\Delta$ ($v = 0$), and $I^1\Sigma^-$ ($v = 0, 1$) rovibrational levels. The comprehensive data set, 281 spectral lines belonging to 3 bands, was included in the fit. The $A^1\Pi$ and perturber states were described in terms of a set of deperturbed molecular constants, spin-orbit and L -uncoupling interaction parameters, individual and equilibrium constants, term values, as well as isotopologue-independent spin-orbit and rotation-electronic perturbation parameters.

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Acknowledgements

R. Hakalla thanks LaserLab-Europe for support of this research (grants: 654148-EUH 2020 and 284464-EC-SFP).

We are grateful to the general and technical staff of SOLEIL for providing beam time under projects no. 20120653 and 20160118.

hakalla@ur.edu.pl



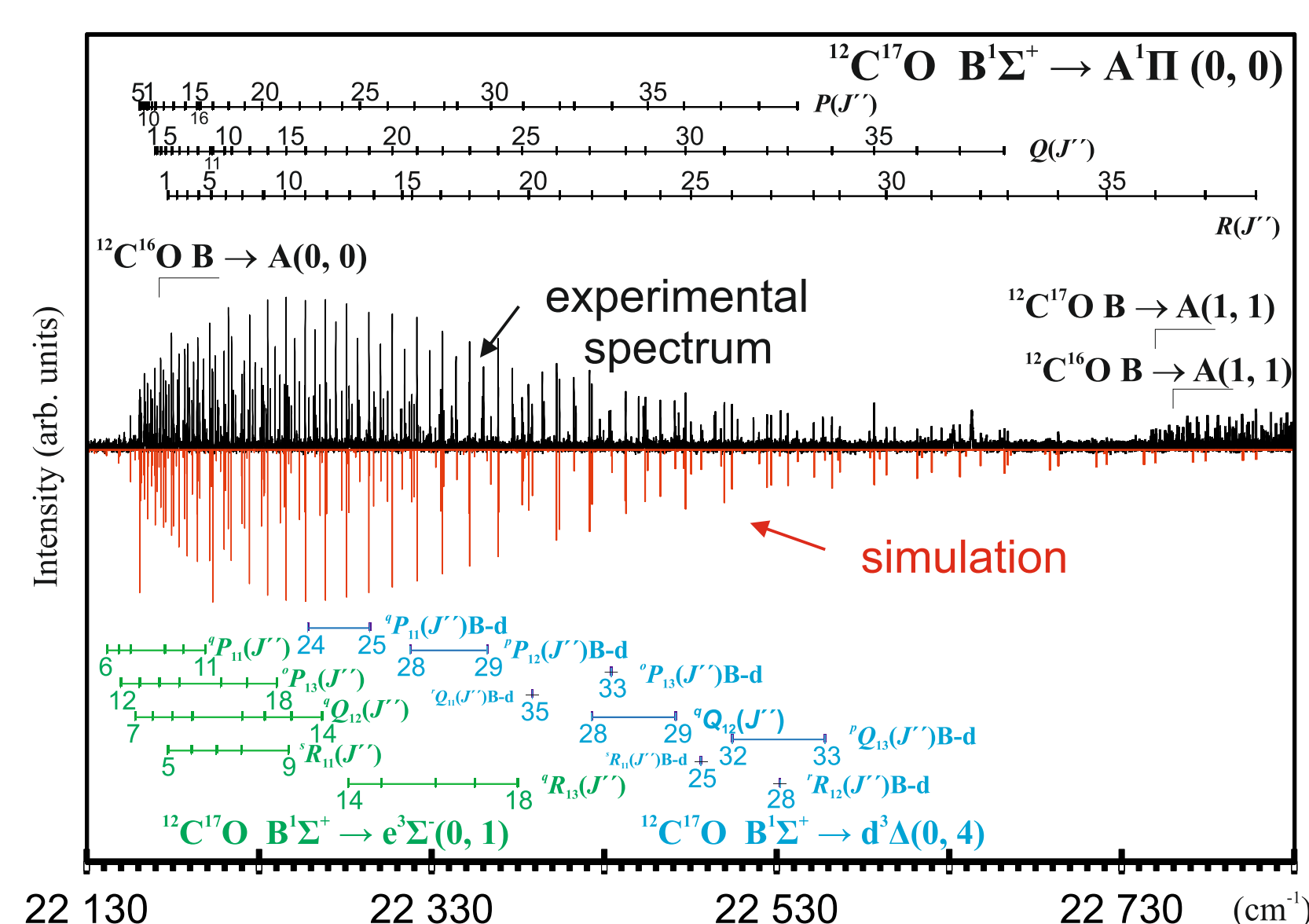
Spectroscopy of Exoplanets
Cumberland Lodge
Windsor Great Park
8 - 11 July 2018

Fourier - transform spectroscopy

LSM Rzeszów

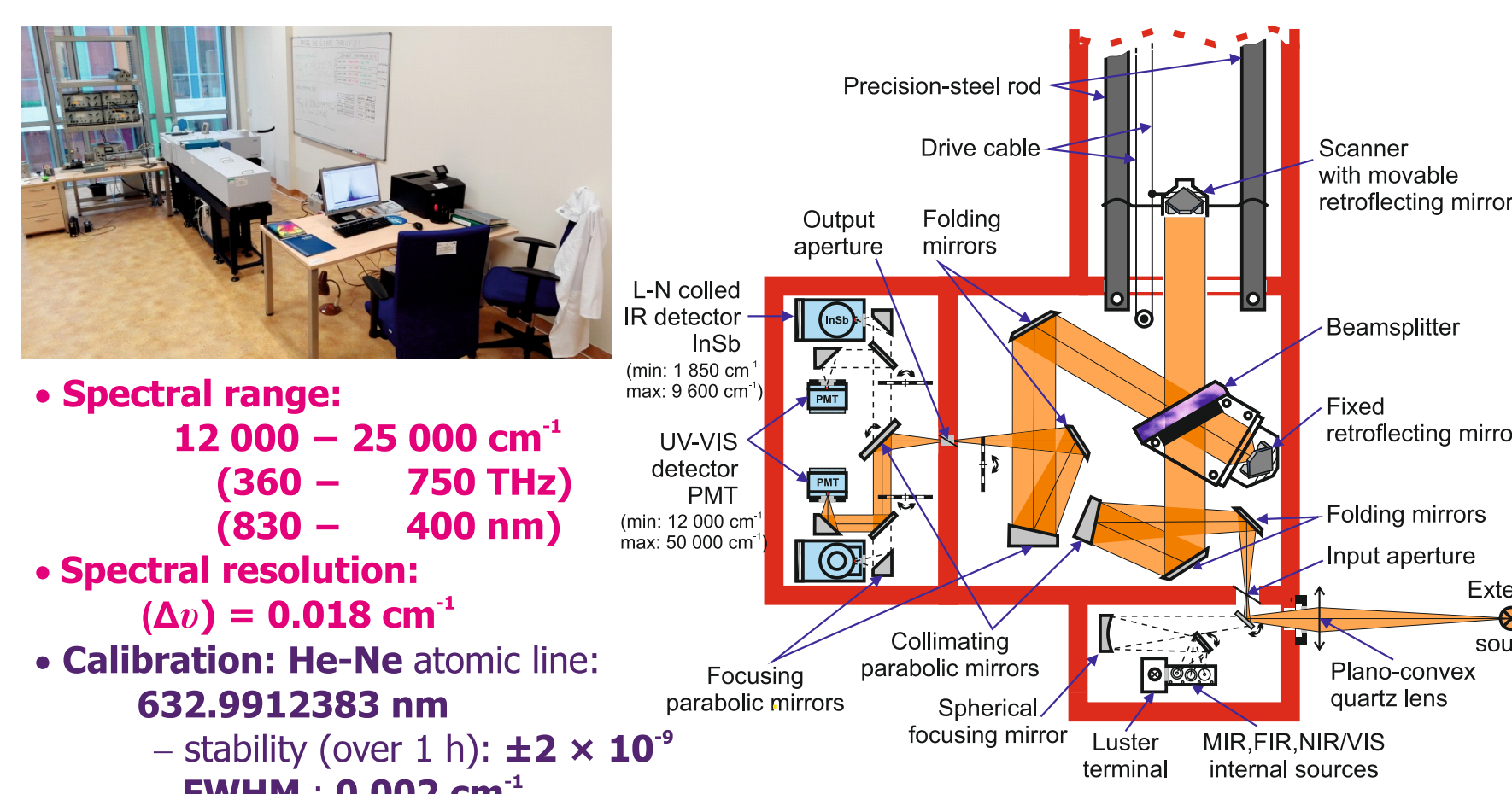
UV-VIS high-resolution emission spectra

$B^1\Sigma^+ \rightarrow A^1\Pi$ (0, 0) of $^{12}\text{C}^{17}\text{O}$



Calibration uncertainty (1 σ): 0.003 cm^{-1}
Accuracy of transition frequencies: 0.005 - 0.03 cm^{-1}

1.71-m spectrometer (Bruker IFS 125HR)

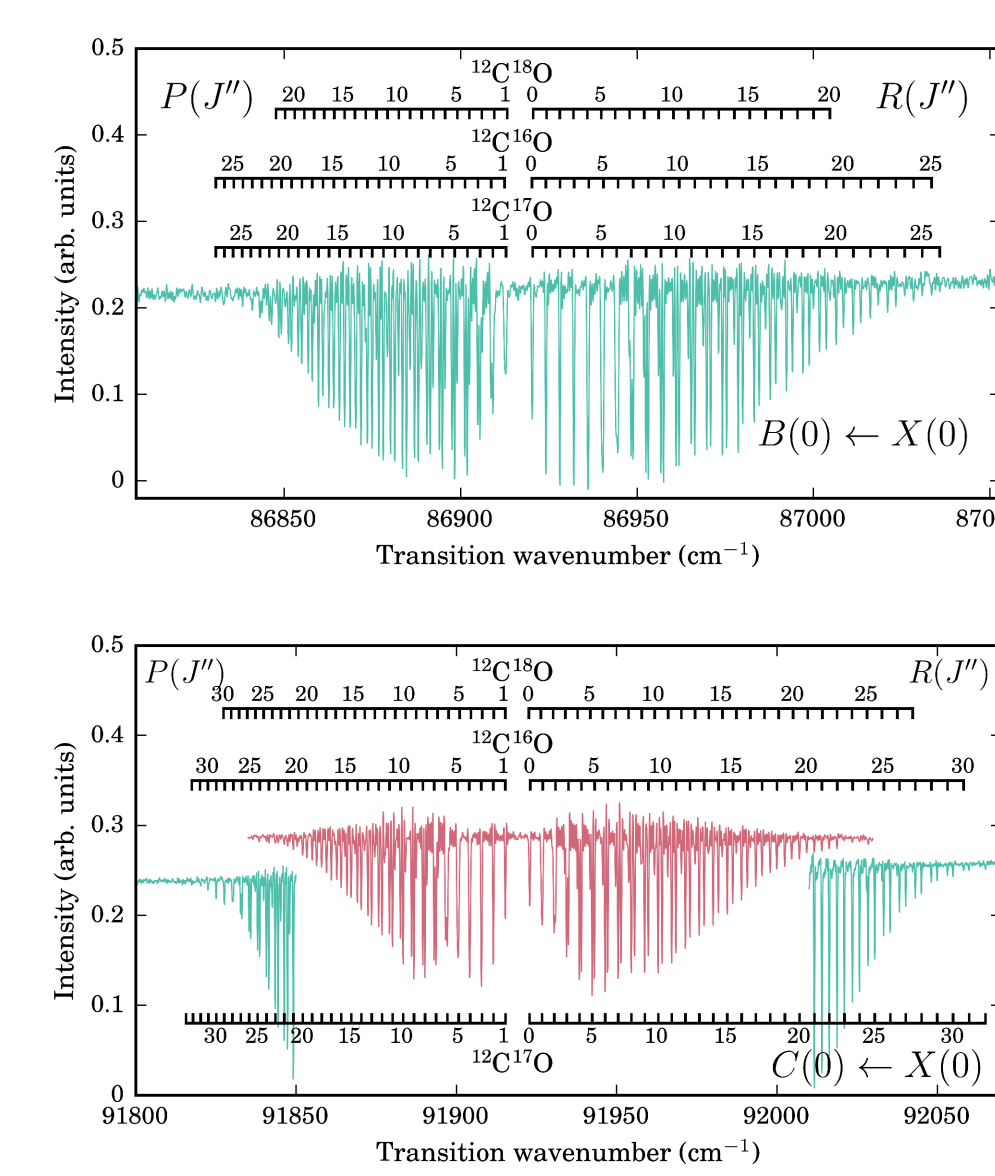


- Spectral range:** 12 000 - 25 000 cm^{-1} (360 - 750 THz) (830 - 400 nm)
- Spectral resolution:** ($\Delta\nu$) = 0.018 cm^{-1}
- Calibration:** He-Ne atomic line: 632.9912383 nm
- stability (over 1 h): $\pm 2 \times 10^{-9}$
- FWHM : 0.002 cm^{-1}

SOLEIL St. Aubin

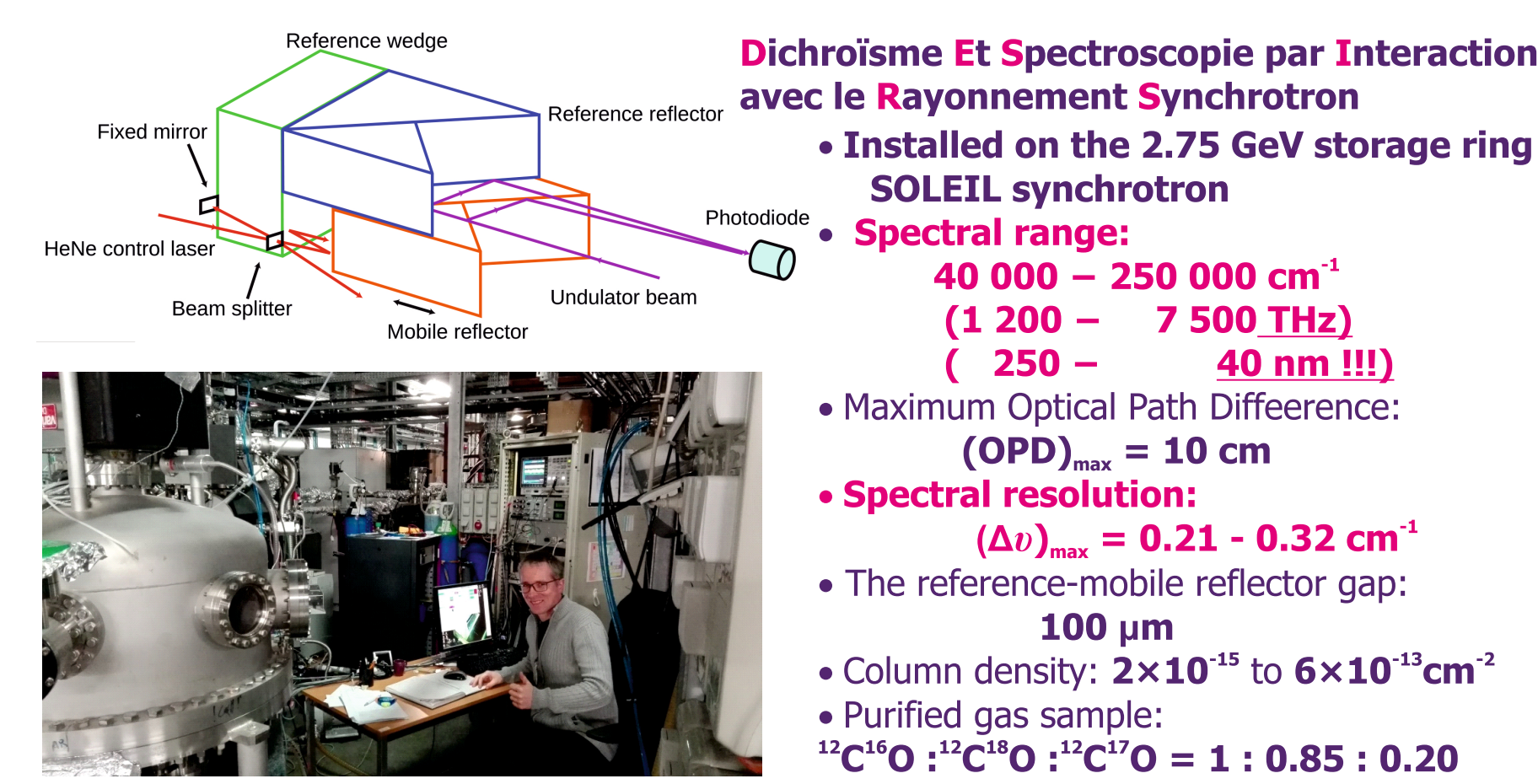
VUV high-resolution absorption spectra

$B^1\Sigma^+ \leftarrow X^1\Sigma^+$ (0, 0) and $C^1\Sigma^+ \leftarrow X^1\Sigma^+$ (0, 0) of $^{12}\text{C}^{17}\text{O}$



Calibration uncertainty (1 σ) : 0.005 cm^{-1}
Accuracy of transition frequencies: 0.01 - 0.1 cm^{-1}

Beamsplitter-less FTS on DESIRS beamline



- Dichroïsme Et Spectroscopie par Interaction avec le Rayonnement Synchrotron**
- Installed on the 2.75 GeV storage ring SOLEIL synchrotron
- Spectral range:** 40 000 - 250 000 cm^{-1} (1 200 - 7 500 THz) (250 - 40 nm !!!)
- Maximum Optical Path Difference: (OPD)_{max} = 10 cm
- Spectral resolution:** ($\Delta\nu$)_{max} = 0.21 - 0.32 cm^{-1}
- The reference-mobile reflector gap: 100 μm
- Column density: 2×10^{15} to $6 \times 10^{13} \text{ cm}^{-2}$
- Purified gas sample: $^{12}\text{C}^{16}\text{O} : ^{12}\text{C}^{17}\text{O} : ^{13}\text{C}^{16}\text{O} = 1 : 0.85 : 0.20$

DEPERTURBATION of the $A^1\Pi$, $v = 0$ level in $^{12}\text{C}^{17}\text{O}$

Constant	$A^1\Pi$ ($v = 0$)	$B^1\Sigma^+$ ($v = 0$)	$C^1\Sigma^+$ ($v = 0$)
T_v	64752.1158(14)	86916.41982(99)	91918.9444(15)
B	1.5635153(72)	1.8989453(40)	1.8945392(78)
$D \times 10^6$	7.0826(48)	6.47 ^b	5.8538(76)
$H \times 10^{11}$	-1.26 ^a		
Constant	$D^1\Delta$ ($v = 0$)	$I^1\Sigma^-$ ($v = 0$)	$I^1\Sigma^-$ ($v = 1$)
T_v	65429.47 ^{d,e}	64552.74 ^{d,f}	65610.06 ^{d,f}
B	1.2167 ^e	1.2290 ^f	1.2121 ^f
$D \times 10^6$	6.69 ^e	6.50 ^f	6.53 ^f
$H \times 10^{12}$	-27.83 ^e	2.59 ^a	2.78 ^a
δ_{calc}	0.026	-0.0425	0.072
Constant	$e^3\Sigma^-$ ($v = 1$)	$d^3\Delta$ ($v = 4$)	$a^3\Sigma^+$ ($v = 9$)
$T_v(F_1)$	64793.9722(16)		65381.16 ^{d,f}
$T_v(F_2)$		65057.9699(30)	
$T_v(F_3)$			
B	1.225661(12)	1.2037550(67)	1.1535 ^f
A		-16.6485(48)	
λ	0.5325(39)	1.095(17)	-1.139 ^f
$\gamma \times 10^3$		-8.13 ^f	
$D \times 10^6$	6.47 ^f	6.15 ^f	5.96 ^f
$H \times 10^{12}$	-1.85 ^a	-0.74 ^a	-0.37 ^a
$A_D \times 10^5$		-4.94 ^f	
η	14.9156(28)	-21.8227(58)	-2.394(29)
η_{calc}	14.822	-21.557	-2.511
δ_{η}^c	0.6	1.2	4.7

In cm^{-1} except δ_{η} . ^a Obtained by isotopic scaling values taken from:
^b Ref. [5], ^c Ref. [2], ^d Ref. [6], ^e [C. Kittrell et al., Spectrochim. Acta 1, 31-40 (1989)], ^f Ref. [3]
^g $\delta_{\eta} = \frac{(\eta_{\text{calc}} - \eta)}{|\eta_{\text{calc}}|} \times 100\%$

$$\begin{aligned} \eta_L &= -a_L \sqrt{3} \\ \zeta_{A-1} &= \beta_{A-1} \sqrt{2} \\ \zeta_{A-D} &= \beta_{A-D} \end{aligned}$$

$$\begin{aligned} a_{A-D} &= \langle A^1\Pi, v_A | H^{SO} | d^3\Delta, v_D \rangle = -(\sqrt{2}/4) a_{A-D} < v_A | v_D \rangle, \quad (1) \\ a_{A-0} &= \langle A^1\Pi, v_A | H^{SO} | e^3\Sigma^-, v_0 \rangle = -(1/4) a_{A-0} < v_A | v_0 \rangle, \quad (2) \\ a_{A-0} &= \langle A^1\Pi, v_A | H^{SO} | a^3\Sigma^+, v_0 \rangle = (1/4) a_{A-0} < v_A | v_0 \rangle, \quad (3) \\ 2\beta_{A-0} \sqrt{J(J+1)} &= \langle A^1\Pi, v_A | H^{RE} | I^1\Sigma^-, v_1 \rangle = -\sqrt{J(J+1)} b_{A-1} < v_A | b_{A-1} \rangle, \quad (4) \\ 2\beta_{A-0} \sqrt{J(J+1)} - 2 &= \langle A^1\Pi, v_A | H^{RE} | D^1\Delta, v_D \rangle = \sqrt{J(J+1)} - 2 b_{A-D} < v_A | b_{A-D} \rangle, \quad (5) \end{aligned}$$

a_L, η_L : spin-orbit interaction parameters;
 β_L, ζ_L : rotational-electronic (L -uncoupling) interaction parameters;
 a, b : spin-orbit and rotational-electronic (L -uncoupling) isotopologue-independent perturbation parameters.

