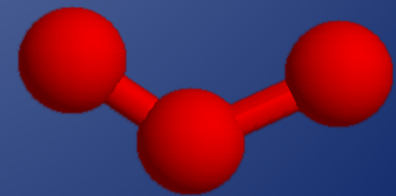


# Ozone Spectroscopic Studies in GSMA, Reims : Results and Outlook

M. Rotger, E. Starikova, A. Barbe, M.-R. De Backer, Vl. G. Tyuterev,  
L. Daumont et G. Durry  
GSMA, Reims

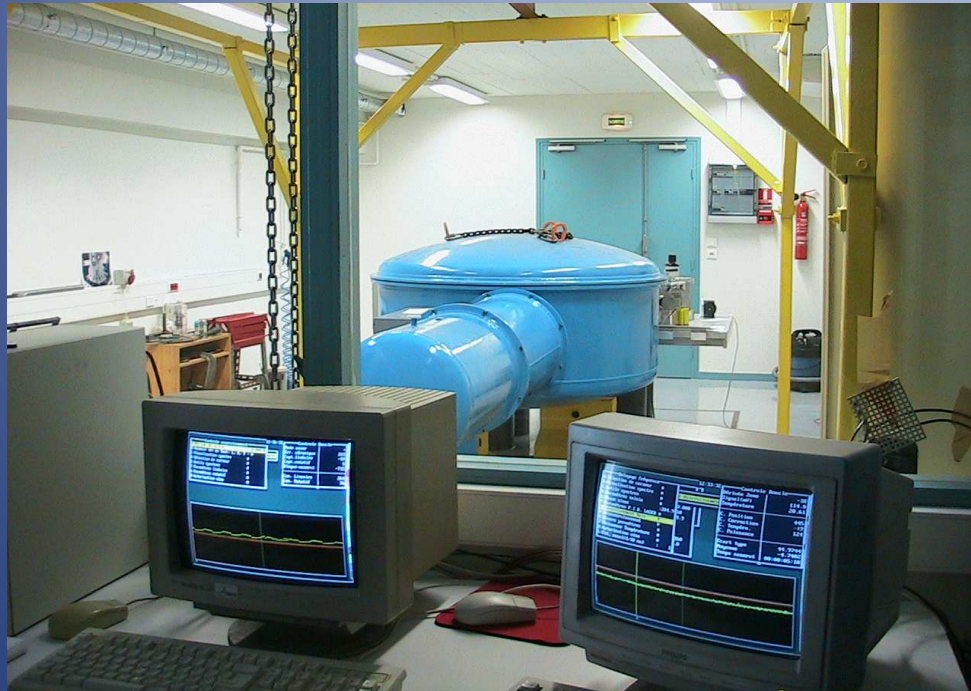


World Meteorological Organization  
Weather • Climate • Water



# FTIR in Reims

Spectral range :  $600 \text{ cm}^{-1} \rightarrow 6000 \text{ cm}^{-1} \Leftrightarrow 1.6 \mu\text{m} \rightarrow 16.5 \mu\text{m}$



Working in stepping mode,  
3 meters path difference.

➤ Frequency calibration

✓ CO, N<sub>2</sub>O, CO<sub>2</sub>, H<sub>2</sub>O

✓ O<sub>3</sub> line :  $24_{1114} \leftarrow 23_{1113}$   
at  $1052.1932396 \text{ cm}^{-1}$  observed by  
saturated absorption ;  $1 \times 10^{-6} \text{ cm}^{-1}$   
précision (Coll. C. Bordé, LPL)

➤ Cells

✓ simple path : 5 cm, 31 cm, 60 cm

✓ White cell: 4.16 m  $\rightarrow$  36.16 m

**Recent experimental improvements:**

➤ Use of two detectors (improved S/N ratio  $\sim$  8000)

➤ Adaptation to large white cell ( 50 m length  $\rightarrow$  1.5 km pathlength )

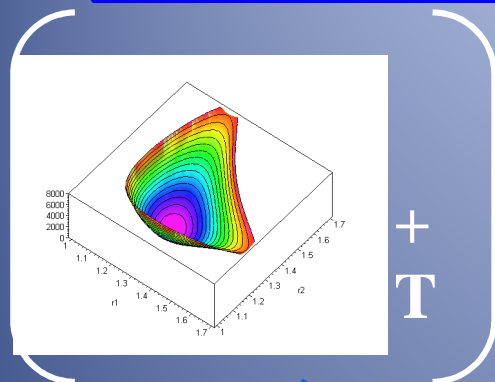
# Ozone Synthesis



- Electric discharge at 400 Hz, 12 000 Volts and 77 K
- Quasi pure ozone (99.9 %)  
 $\Rightarrow P(\text{O}_3) = 2(P_{\text{init}}(\text{O}_2) - P_{\text{fin}}(\text{O}_3 + \text{O}_2))$
- $^{16}\text{O}_2$  and  $^{18}\text{O}_2$  mixture  $\Rightarrow$  6 isotopologues

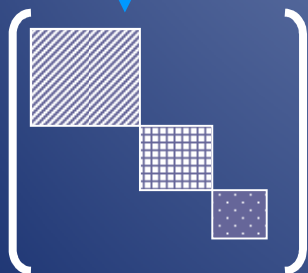


# Line by line simulation



+ T

Perturbative theory (CT)



Effective Hamiltonian with calculated parameters

Direct calculations

Diagonalisation

$E_n^{calc}$



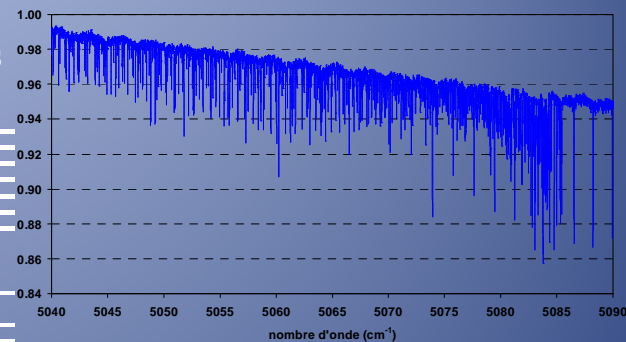
$E_n^{obs}$



Comparison

Comparison

Absorption Spectrum



- Molecules
- Cell length
- Temperature
- Pression

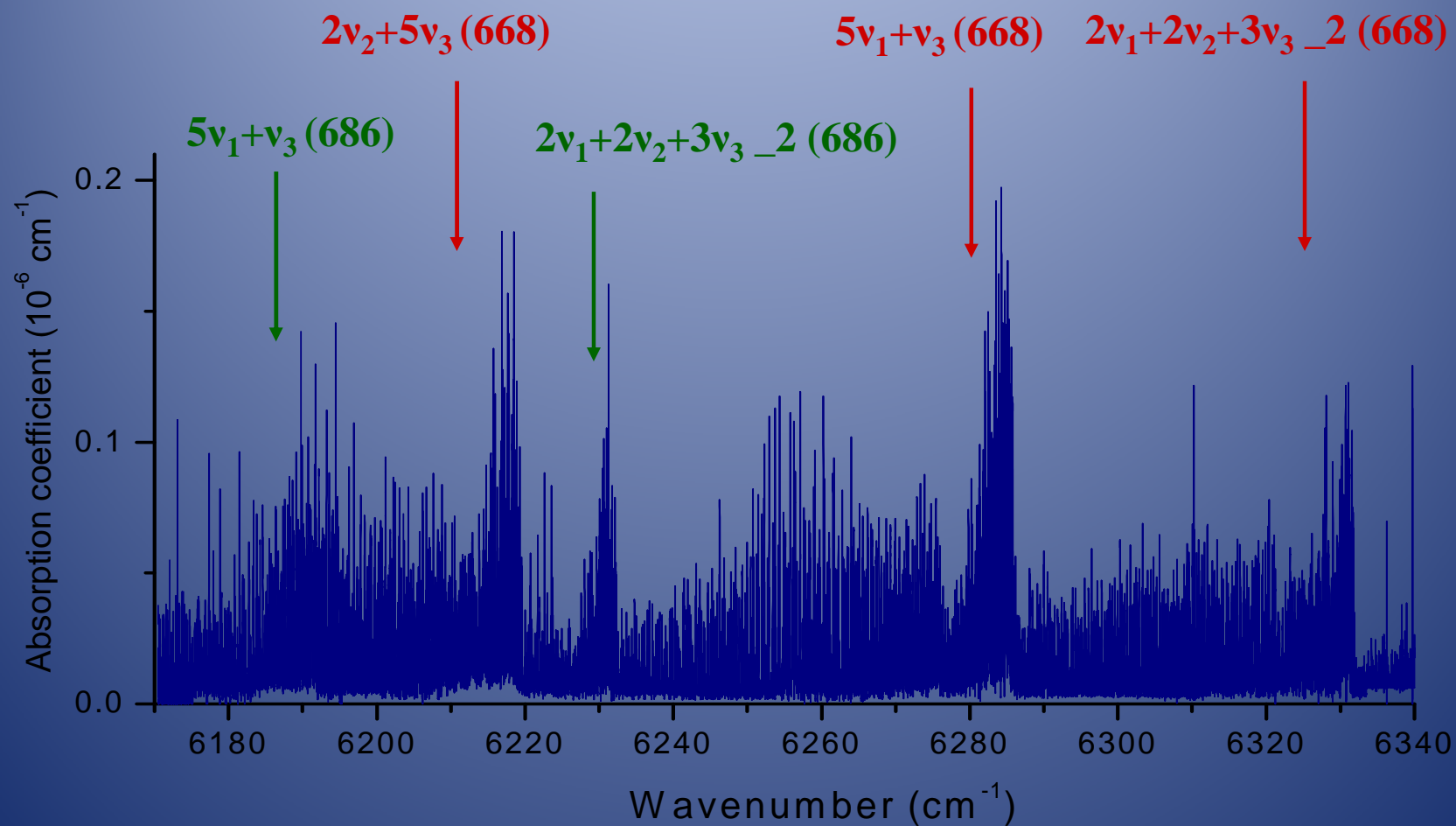
Assignments

Modelisation

- Positions
- Intensities

Effective Hamiltonian with empirical parameters

# CRDS in Grenoble



Exp. : A. Campargue *et al.*, LIPhy, Grenoble

ACSO Meeting, Genève, June 3-5 2013

## $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ : Recent Analyses -- 20 bands

	Band	Observed	Obs.-Calc. ( $\text{cm}^{-1}$ )	J max	$K_a$ max	Nbr of transitions	RMS ( $\times 10^{-3} \text{ cm}^{-1}$ )
(223)_1	$2\nu_1+2\nu_2+3\nu_3-1$	5983.628	-0.356	27	9	356	4.9
(025)	$2\nu_2+5\nu_3$	6151.381	-0.277	31	10	416	7.8
(501)	$5\nu_1+\nu_3$	6182.305	-0.199	30	9	353	
(223)_2	$2\nu_1+2\nu_2+3\nu_3-2$	6225.259	0.064	27	6	260	13.1

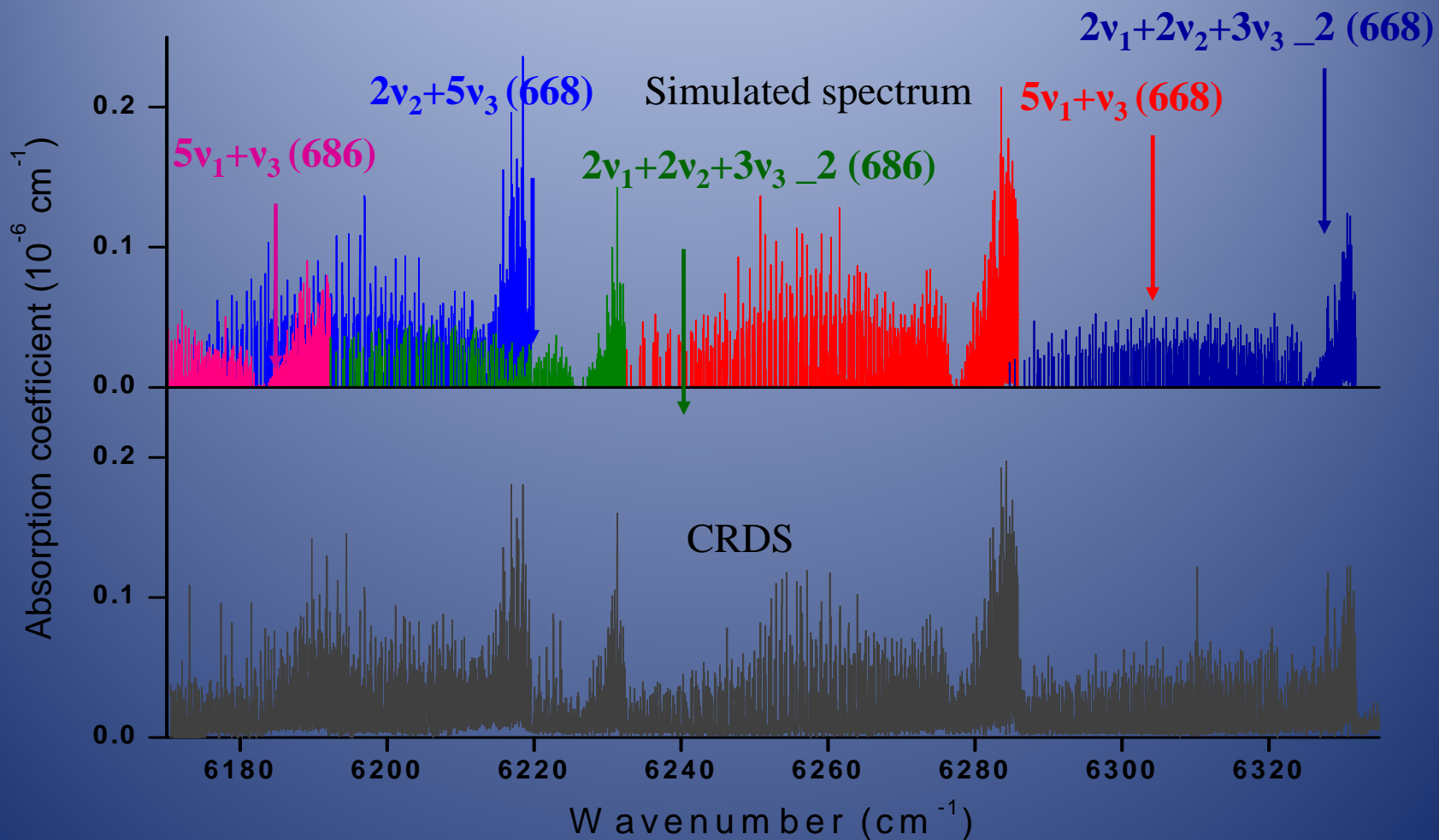
## $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ : Recent Analyses -- 24 bands

	Band	Observed	Obs.-Calc. ( $\text{cm}^{-1}$ )	J max	$K_a$ max	Nbr of transitions	RMS ( $\times 10^{-3} \text{ cm}^{-1}$ )
(102)	$\nu_1+2\nu_3$	3060.565	-0.034	35	5	234	
(201)	$2\nu_1+\nu_3$	3148.145	+0.073	36	12	465	1.38
(121)	$\nu_1+2\nu_2+\nu_3$	3403.670	-0.087	24	11	172	14.8
(013)	$\nu_2+3\nu_3$	3636.934	-0.019	25	10	206	2.37
(004)	$4\nu_3$	3932.992	+0.039	28	11	245	
(103)	$\nu_1+3\nu_3$	4002.412	-0.083	37	14	424	5.72
(202)	$2\nu_1+2\nu_3$	4092.467	+0.043	29	10	234	
(113)	$\nu_1+\nu_2+3\nu_3$	4624.318	-0.131	15	8	78	18
(005)	$5\nu_3$	4824.383	+0.169	32	11	246	2.79
(223)_1	$2\nu_1+2\nu_2+3\nu_3-1$	6026.084	-0.047	24	11	556	4.9
(025)	$2\nu_2+5\nu_3$	6213.492	-0.072	29	8	498	7.53
(501)	$5\nu_1+\nu_3$	6276.706	0.000	32	9	601	10.2
(223)_2	$2\nu_1+2\nu_2+3\nu_3-2$	6325.214	-0.163	27	10	505	5.35

## $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ : 21 bands and $^{18}\text{O}^{18}\text{O}^{16}\text{O}$ : 19 bands

ACSO Meeting, Genève, June 3-5 2013

# Absorption near the dissociation



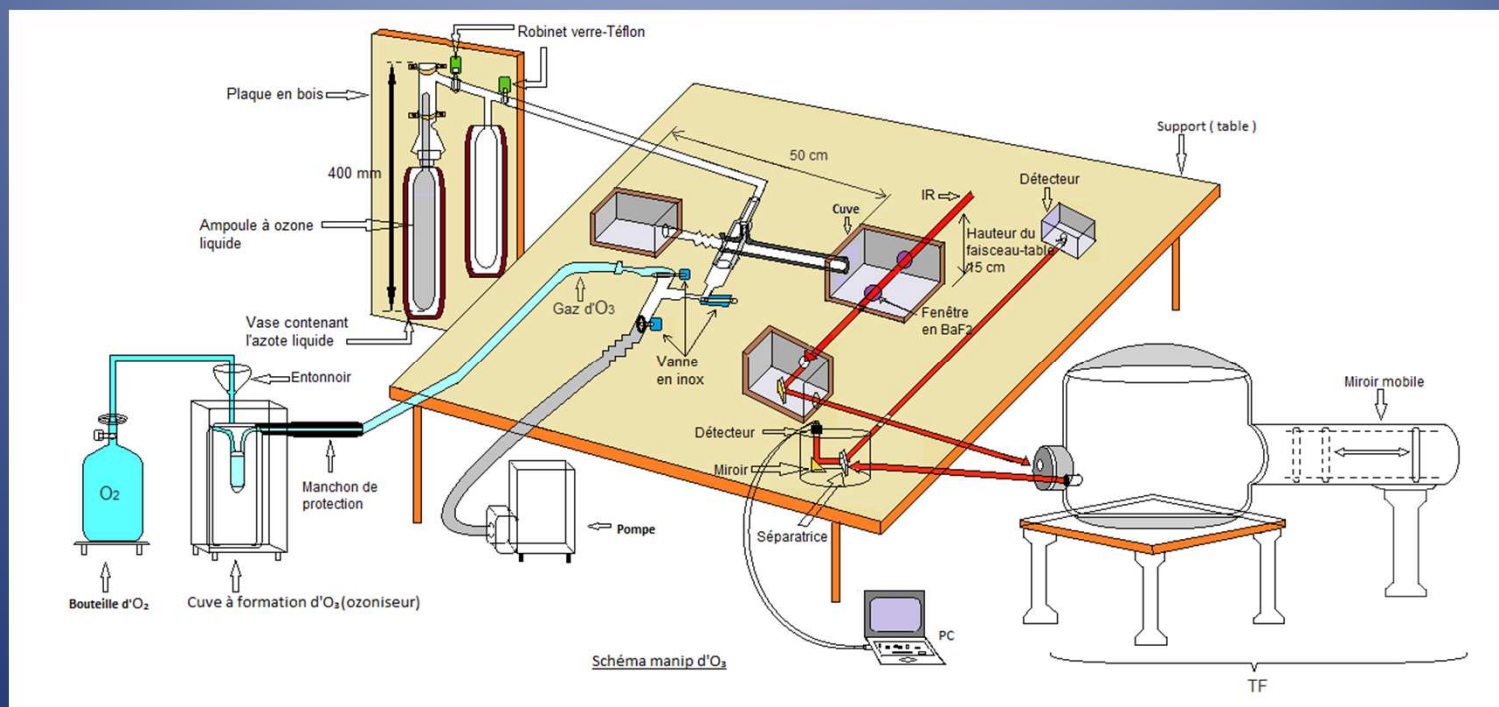
# Outlook

## **New High-Resolution Bruker FT Spectrometer in Reims**

- UV cross-sections measurements at low temperature (Huggins band) using a liquid nitrogen cooling White cell developed for methane applications
- Intensities measurements at 10 and 5  $\mu\text{m}$
- Inter-comparison between IR (home-made FTIR) and UV (Bruker) measurements



# ANR@IDEO : $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ at Reims : Absolute Intensities



I. Diallo, M.-R. De Backer, M. Rotger

ACSO Meeting, Genève, June 3-5 2013

# ANR@IDEO : $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ at Reims

- **Test all the set-up to vacuum**
- **Passivation of the set-up with ozone  $^{16}\text{O}^{16}\text{O}^{16}\text{O}$**
- **Simulations of  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$  spectra for the  $\nu_1$  and  $\nu_1 + \nu_3$  bands**
- **Recordings of the  $\nu_1$  band at  $10\ \mu\text{m}$  ( $P = 1\ \text{Torr}$  ;  $L = 5,7\ \text{cm}$ )**
- **Recordings of the  $\nu_1 + \nu_3$  band at  $5\ \mu\text{m}$  ( $P = 6,5\ \text{Torr}$  ;  $L = 5,7\ \text{cm}$ )**

Welcome in Reims  
at the Best Western  
« Hôtel de La Paix »

Chairs :  
Vi. Tyuterev  
M. Rotger

Accueil > Homepage

Homepage  
First circular  
Registration

Moteur de recherche : Mots clés... Rechercher

## OZONE WORKSHOP 2013



2<sup>nd</sup> International WORKSHOP  
“Spectroscopy and Dynamics of  
Ozone and Related Atmospheric  
Species”  
REIMS, FRANCE, October 2-4,  
2013

Logos: CNRS, SPECMO, Eur planet, A, GSMA, CHAMPAGNE ARDENNE, MGEN, casden

<http://www.univ-reims.fr/site/evenement/ozone-2013/homepage,14120,24526.html>