



## 3-d International WORKSHOP “Spectroscopy and Dynamics of Ozone and Related Atmospheric Species” REIMS, FRANCE, October 4-6, 2017

Wednesday, October 4		workshop schedule	
	10:30 - 12:00	<b>Arrival / Registration</b>	
	12:15 – 13:45	Lunch	
	14:15 – 14:30	Opening	
<b>Ozone theory</b>  Chair: O.Dulieu	14:30 – 15:10	W1 - R. Dawes	Investigation of the ozone formation reaction pathway: Comparisons of Full Configuration Interaction Quantum Monte Carlo and Fixed-Node Diffusion Monte Carlo with contracted and uncontracted MRCI
	15:15 – 15:45	W2 - V. Kokoouline	Spectroscopic and dynamical properties of the ozone molecule in the dissociation region
	15:50 – 16:10	W3 - D. Lapiere	Predissociation resonances of O <sub>3</sub>
	16:15	End of session	
	16:15	Coffee break	
<b>Ozone theory and dynamics</b>  Chair: V.Kokoouline	16:45 – 17:05	W4 - S. Ndengué	Resonance and inelastic scattering calculations to understand the ozone isotopic anomaly
	17:10 – 17:30	W5 - C. Janssen	Mass independent isotope effects in simple triatomic reactions
	17:35 – 18:15	W6 - V. Tyuterev	Ab initio dipole moment surfaces of ozone: variational predictions of line intensities for isotopic species and comparison with experiments
	18:20	End of session	
	19:30	<b>Banquet</b> at Restaurant “Excelsior” (ancien Brasserie “Flo”) 96 place Drouet d’Erlon	

*5 min are left after each talk for questions and discussions*

Buffet Lunches take place at the restaurant of Hotel de la Paix

Thursday, October 5		workshop schedule	
<b>Ozone dynamics</b> Chair: R.Dawes	9:15 – 9:35	T1 - G. Guillon	Permutation symmetry in quantum dynamics: examples with O + O <sub>2</sub> reactions
	9:40 – 10:20	T2 - P. Honvault	Quantum dynamics study of the O + O <sub>2</sub> collisions
	10:25	End of session	
	10:25 – 10:55	Coffee break	
<b>Ozone spectroscopy</b>	10:55 – 11:15	T3 - A. Barbe	Analyses of <sup>17</sup> O isotopic species of ozone in the 5 and 10 microns spectral ranges
	11:20 – 11:40	T4 - E. Starikova	FTS high resolution spectra of <sup>16</sup> O <sup>16</sup> O <sup>18</sup> O in 900-3500 cm <sup>-1</sup> range: Analyses and theoretical modeling for the polyads of coupled states.
	11:45 – 12:05	T5 - D. Mondelain	Highly excited levels of the <sup>16</sup> O/ <sup>18</sup> O ozone isotopologues by CRDS near the dissociation energy
	12:10	End of session	
	12:15 - 13:45	Lunch	
<b>Atmosphere</b> Chair: C.Janssen	14:00 – 14:40	T6 - J. Cuesta	Satellite observation of lowermost tropospheric ozone by multispectral synergism of IASI thermal infrared and GOME-2 ultraviolet measurements
	14:45 – 15:20	T7 – H. Tran	Line-shape problems in modelling laboratory and atmospheric spectra
	15:25 – 15:55	T8 - V. Yankovsky	Model of electronic-vibrational kinetics of the products of ozone and molecular oxygen photodissociation in the mesosphere and lower thermosphere of the Earth
	16:00	End of session	
	16:00	Coffee break	
<b>Ozone spectroscopy and atmosphere</b> Chair: A.Perrin	16:30 -16:45	T9 - M. Minissale	Non-linear frequency-sweep correction of quantum cascade lasers and laser based shift measurement of molecular lines of ozone at 9.54 μm
	16:50 – 17:05	T10 - C. Janssen	New quantitative ozone spectroscopic studies over multiple spectral regions
	17:10 – 17:25	T11 - S. Mikhailenko	Study of the (004) / (103) / (310) ozone system: current status
	17:30 – 17:45	T12 - M.-R. De Backer	Ozone absorption cross-section measurements in the UV-Hartley band
	17:50 – 18:05	T13 - M. Zoran	Temporal patterns of surface ozone levels and its relation with radon ( <sup>222</sup> Rn) and air quality
	18:10 – 18:25	T14 - C. Kalalian	Gas phase reaction of ozone with C5 and C6 unsaturated aldehydes and alcohols
	18:30	End of session	
	19:00	Réception at the Mairie de Reims (Reims Town hall )	

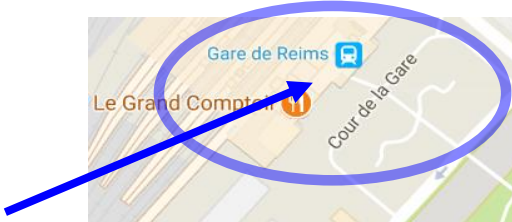
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Friday, October 6 workshop schedule			
<b>Databases</b> Chair: A.Barbe	9:05 – 9:35	F1 - V. Gorshlev	Updated ozone absorption cross-sections in the Huggins band
	9:40 – 10:10	F2 - R. Armante	From GEISA-2015 to GEISA-2018: ozone content and validation
	10:15	End of session	
	10:15 – 10:45	Coffee break	
<b>Databases</b>	10:45 – 11:15	F3 - I. Gordon	HITRAN 2016 database: Reference atmospheric spectroscopy boosted by data science
	11:20 – 11:40	F4 - V. Boudon	Molecular Spectroscopy Databases in the Framework of the VAMDC and DAT@OSU Projects
	11:45 – 12:05	F5 - M. Rey	TheoReTS: ab initio-based Reims-Tomsk database for atmospheric, planetological and astrophysical applications
	12:10	End of session	
	12:15 – 13:45	Lunch	
<b>Other molecules</b> Chair: M.Rotger	14:15 – 14:35	F6 - A. Perrin	Investigation of the $\nu_8$ and $\nu_{21}$ bands of propane $\text{CH}_3\text{CH}_2\text{CH}_3$ at 870.348 and 921.382 $\text{cm}^{-1}$ : evidence of large amplitude tunnelling effects.
	14:40 – 14:55	F7 - E. Neeman	The quasi-unchanged structure of monoterpenes and their oxidation products
	15:00 – 15:15	F8 - M. Mattoussi	Analysis of the $(\nu_2+2\nu_4, \nu_2+\nu_3, 4\nu_2, \nu_1+2\nu_2, 2\nu_1)$ pentad of $\text{CF}_4$
	15:20 – 15:35	F9 - A. Boughdiri	Frequency analysis of the $(\nu_2/\nu_3 + \nu_6/\nu_5/3\nu_3)$ tetrad of $\text{CH}_3\text{I}$
	15:40 – 15:55	F10 - O. Ferchichi	Ab initio structural analysis of peroxide molecules: $\text{CH}_3\text{OOCH}_3$ and $\text{ClOOCl}$
	16:00	End of session	<b>Workshop closing</b>
	16:15	Coffee break	
		Departure	

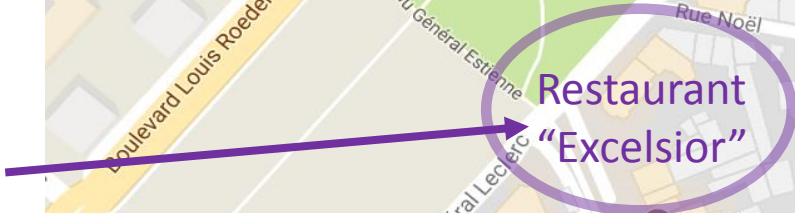
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# REIMS city center

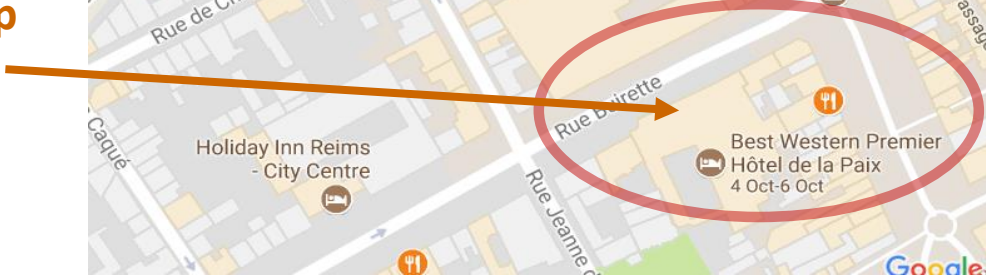
**Cental railway station**



**Banquet Wednesday evening**



**Workshop venue**



**Reception Thursday evening**

