

Workshop Program

Spectroscopy and Dynamics of Ozone and Related Atmospheric Species

Reims, October 4 – 6, 2017



OZONE workshop

The banner features a dark blue background with a light blue horizon line. It includes several scientific illustrations: three purple and blue spheres on the left, a green and blue wave pattern, a central 3D bar chart with orange peaks, and another green and blue wave pattern on the right. A red and white bar chart is positioned at the bottom left. Logos for CNRS, GSMA, Reims, and Université de Reims Champagne-Ardenne are located at the bottom.

Reims, 4 – 6 October 2017

CNRS **GSMA** **Reims** **UNIVERSITÉ DE REIMS CHAMPAGNE-ARDENNE**

Wednesday October 4, 2017

Afternoon session: "Ozone Theory"

W1 - 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

R. Dawes

W2 - Spectroscopic and dynamical properties of the ozone molecule in the dissociation region

V. Kokoouline, A. Alijah, R. Kochanov, D. Lapierre, V. Tyuterev

W3 - Predissociation resonances of O₃

D. Lapierre, A. Alijah, R. Kochanov, V. Kokoouline, V. Tyuterev

Afternoon session: "Ozone Theory and Dynamics"

W4 - Resonance and inelastic scattering calculations to understand the ozone isotopic anomaly

S. Ndengué

W5 - Mass independent isotope effects in simple triatomic reactions

D. Simone, L.M. Joelsson, M.S. Johnson, M. Minissale, P. Jeseck, T. Zanon, C. Janssen

W6 - Ab initio dipole moment surfaces of ozone: variational predictions of line intensities for isotopic species and comparison with experiments

V. Tyuterev, R. Kochanov, S. Tashkun, A. Barbe

Thursday October 5, 2017

Morning session: "Ozone Dynamics"

T1 - Permutation symmetry in quantum dynamics: examples with O + O₂ reactions

G. Guillon, P. Honvault

T2 - Quantum dynamics study of the O + O₂ collisions

P. Honvault, G. Guillon

Morning session: "Ozone Spectroscopy"

T3 - Analyses of ¹⁷O isotopic species of ozone in the 5 and 10 microns spectral ranges

A. Barbe, M.-R. De Backer, V. Tyuterev, E. N. Starikova

T4 - FTS high resolution spectra of $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ in 900-3500 cm^{-1} range: Analyses and theoretical modeling for the polyads of coupled states.

A. Barbe, M.-R. De Backer, V. Tyuterev, E. N. Starikova

T5 - Highly excited levels of the $^{16}\text{O}/^{18}\text{O}$ ozone isotopologues by CRDS near the dissociation energy

D. Mondelain, A. Campargue, S. Kassi

Afternoon session: "Atmosphere"

T6 - Satellite observation of lowermost tropospheric ozone by multispectral synergism of IASI thermal infrared and GOME-2 ultraviolet measurements

J. Cuesta, M. Eremenko, X. Liu, G. Dufour, G. Foret, A. Coman, Z. Cai, M. Beekmann, M. Höpfner, T. von Clarmann, J. Orphal, K. Chance and J.-M. Flaud

T7 - Line-shape problems in modelling laboratory and atmospheric spectra

H. Tran

T8 - Model of electronic-vibrational kinetics of the products of ozone and molecular oxygen photodissociation in the mesosphere and lower thermosphere of the Earth

V. Yankovsky

Afternoon session: "Ozone Spectroscopy and Atmosphere"

T9 - Non-linear frequency-sweep correction of quantum cascade lasers and laser based shift measurement of molecular lines of ozone at 9.54 μm

M. Minissale, T. Zanon-Willette, I. Prokhorov, H. Elandaloussi, P. Jeseck, C. Boursier, C. Janssen

T10 - New quantitative ozone spectroscopic studies over multiple spectral regions

C. Janssen, H. Elandaloussi, P. Jeseck, C. Boursier, Y. Té, J. Gröbner

T11 - Study of the (004) / (103) / (310) ozone system: current status

A. Barbe, S. Mikhailenko

T12 - Ozone absorption cross-section measurements in the UV-Hartley band

G. Alhora, A. Alkadrou, M.-R. De Backer, B. Grouiez, M. Rotger, L. Daumont, N. De Oliveira, K. Ito, D. Joyeux

T13 - Temporal patterns of surface ozone levels and its relation with radon (^{222}Rn) and air quality

M. Zoran, D. Savastru, A. Dida

T14 - Gas phase reaction of ozone with C5 and C6 unsaturated aldehydes and alcohols

C. Kalalian, E. Roth, A. Chakir

Friday October 6, 2017

Morning session: "Databases"

F1 - Updated ozone absorption cross-sections in the Huggins band
V. Gorshelev, M. Weber, J. P. Burrows

F2 - From GEISA-2015 to GEISA-2018: ozone content and validation
R. Armante, N. Jacquinet, A. Perrin, N. Scott, A. Chédin, L. Crépeau

Morning session: "Databases" (continued)

F3 - HITRAN 2016 database: Reference atmospheric spectroscopy boosted by data science
E. Gordon, L. S. Rothman, R.V. Kochanov, Y. Tan, C. Hill, and HITRAN contributors worldwide

F4 - Molecular Spectroscopy Databases in the Framework of the VAMDC and DAT@OSU Projects
V. Boudon, C. Richard, M. Rotger

F5 - TheoReTS: *ab initio*-based Reims-Tomsk information system for atmospheric, planetological and astrophysical applications
M. Rey, A. Nikitin, Y. Babikov, I. Chizhmakova, A. Rodina, E. Starikova, D. Viglaska, V. Tyuterev

Afternoon session: "Other molecules"

F6 - Investigation of the ν_8 and ν_{21} bands of propane $\text{CH}_3\text{CH}_2\text{CH}_3$ at 870.348 and 921.382 cm^{-1} : evidence of large amplitude tunnelling effects.
A. Perrin, J-M Flaud, F. Kwabia-Tchana, L. Manceron, P. Groner

F7 - The quasi-unchanged structure of monoterpenes and their oxidation products
E. M. Neeman, M. Chrayteh, P. Drean, T. R. Huet

F8 - 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 CF_4
M. Mattoussi, M. Rey, A.V. Nikitin, I. Chizhmakova, M. Rotger, H. Aroui, S. Tashkun, V. Tyuterev

F9 - Frequency analysis of the $(\nu_2/\nu_3+\nu_6/\nu_5/3\nu_3)$ tetrad of CH_3I
A. Boughdiri, M. Rey, A. Nikitin, M. Rotger, L. Manceron, H. Aroui

F10 - Ab initio structural analysis of peroxide molecules: CH_3OOCH_3 and ClOOCl
O. Ferchichi, N. Derbel, N. Jaidane, T. Cours, A. Alijah