

WORKSHOP

“Spectroscopy and dynamics of ozone and related atmospheric species”

REIMS, FRANCE, 2-4 October 2013

Program: corrected version of 01/10/2013

===== **Wednesday, 2 october** =====

13h00 : lunch (Hôtel de la Paix)

15h00 : *Workshop opening*

Session A. chairman : A.Campargue

15h15 – 15h45 : The High-Resolution CRDS absorption spectrum of the $^{16}\text{O}/^{18}\text{O}$ ozone isotopologues close to the dissociation energy (5850-7920 cm^{-1}), D. Mondelain, A. Campargue, S. Kassi, R. Jost

15h50– 16h10 : FTIR Experiments in Reims: Past and Future, M. Rotger, X. Thomas, M.-R. De Backer, A. Barbe

16h15 – 16h45 : Coffee break

16h45 – 17h30 : Analyses of High-resolution infrared spectra of ozone recorded by FTS and CRDS, including all ^{18}O enriched isotopologues. Review of the recent results, A. Barbe, M.-R. De Backer, E.N. Starikova

17h35 – 18h20 : Updates on ozone absorption cross sections and intensities : From UV (253.65 nm) to IR (10 μm) spectral régions, C. Janssen, D. Simone, M. Guinet, H. Elandaloussi, C. Camy-Peyret, D. Mondelain, P. Jeseck, Y.V. Té

19h30 : Workshop Dinner : Restaurant « Côté Cuisine »

===== **Thursday, 3 October** =====

Session B . chairman : O.Dulieu

9h00 – 9h35 : Accurate description of potential energy surfaces by ab initio methods : a review and application to ozone, P.G. Szalay, T. Müller, Vl.G. Tyuterev

9h40 – 10h25 : New potential energy surface for the ozone electronic ground state and accurate vibration predictions for spectroscopy at high energy range, Vl.G. Tyuterev, R.Kochanov, S.Tashkun, P.G. Szalay

10h30 – 11h00 : Coffee break

11h00 – 11h45 : The Multi-Configuration Time-Dependent Hartree (MCTDH) Method. Possible Applications to Ozone, F. Gatti

Ozone Photolysis : Strong Isotopologue/Isotopomer Selectivity in the Stratosphere, F. Gatti, S. Ndengué, R. Jost

11h50 – 12h10 : Long-range interactions in the ozone molecule : spectroscopic and dynamic points of view, M. Lepers, B. Bussery-Honvault, O. Dulieu

12h15 : lunch (Hôtel de la Paix)

Session C . chairman : J.Orphal

14h15 – 15h00 : A new global potential energy surface for the ground state of ozone based on explicitly-correlated MRCI-F12 ab initio data , R. Dawes

15h05 – 15h25 : Experimental and Modelling Studies of Anomalous Oxygen Isotope Effects in the Formation of Carbon Dioxide from Irradiated Mixtures of Carbon Monoxide and Ozone or Oxygen – evidence for the spin-forbidden process $O_3 + hv \rightarrow O(1D) + O_2$ at wavelengths larger than 380 nm, D. Simone, C. Janssen, LMT Joellson, MS Johnson

15h30 – 15h50 : Terahertz rotational spectroscopy of atmospheric molecules, R.Motienko, L.Margulès, O.Zakharenko, T.Huet

16h00 – 16h30 : Coffee break

16h40 – 18h00 : ANR IDEO meeting

18h30 : R. LEHOUCQ. Conférence grand public « Peut-on parler de physique grâce à la science-fiction ? » (Hôtel de Ville)

===== **Friday, 4 october** =====

Session D. chairman : C. Janssen

8h45 – 9h30 : Ozone : challenges for the next century, J. Orphal

9h35 – 10h00 : Infrared radiation of ozone in the mesosphere and lower thermosphere: energetic effects and remote sensing, A.G. Feofilov , A.A. Kutepov , and L. Rezac

10h05 – 10h25 : Ozone vertical columns over Paris (Créteil-France) : diurnal and seasonal variations and comparison with correlative satellite and in situ observations, P. Chelin, C. Viatte, M. Eremenko, M. Ray , J. Cuesta, F. Hase, J. Orphal, J.-M. Flaud

10h30 – 11h00 : Coffee break

Session E. chairman : A.Barbe

11h00 – 11h20 : On the origin of mass-independent fractionation of oxygen isotopes in the ozone forming recombination reaction, M.V. Ivanov and D. Babikov

11h25 – 11h45 : Spectroscopy and Molecular Properties of Ozone (S&MPO) information system : state of art and critical issues, S.N. Mikhailenko, A. Barbe, Yu. L. Babikov, Vl.G. Tyuterev

11h50 – 12h10 : GEISA 2013 Ozone and related atmospheric species contents description and assessment, N. Jacquinet-Husson, C. Boutamine, R. Armante, L. Crépeau, A. Chédin, N. Scott, C. Crevoisier, V. Capelle

12h15 : lunch (Hôtel de la Paix)

Afternoon: end of the Workshop / departure