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Observatory for Astrochemical Kinetics and Related Aspects

VINCENZO AQUILANTI[1] – ANDREA LOMBARDI[2] – FEDERICO PALAZZETTI[3]

[1] Uno dei XL. Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, 06123, Perugia, Italy e Istituto di Struttura della materia, Consiglio Nazionale delle Ricerche, Roma, Italy. E.mail: vincenzo.aquilanti@yahoo.it
[2] Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, 06123, Perugia, Italy. E.mail: ebiu2005@gmail.com
[3] Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, 06123, Perugia, Italy. E.mail: federico.palazzetti@unipg.it

Abstract – The articles collected in this issue are contributions prepared on the occasion of a Conference that has been held at the Library of the Italian National Academy of Sciences (said of the Forty) in the *Scuderie Vecchie* of Villa Torlonia in Rome. The meeting follows a series of periodic events hosted by the Academy and organized as an activity of Center for Studies dedicated to astrophysics and astrochemistry; it has taken place on 27 and 28 June 2019. The chosen topic was on aspects related to astrochemical kinetics, celebrating 160 years from Arrhenius birthday and 130 years of remarkable success of his equation: the open problems on its foundations, the current state-of-the-art and the perspectives of future applications were under focus.

Keywords: Chemical Reactions; Theory and Experiments; Kinetics and Statistical Mechanics; Astrophysical, Astrochemical, Astrobiological Modeling

Riassunto – Gli articoli raccolti in questo fascicolo sono contributi che sono stati preparati in occasione di un Convegno che si è tenuto presso la Biblioteca dell'Accademia Nazionale delle Scienze, detta dei Quaranta, nelle Scuderie Vecchie di Villa Torlonia a Roma. L'incontro segue una serie di eventi periodici ospitati dall'Accademia e organizzati come attività del Centro Studi dedicato all'astrofisica e all'astrochimica: si è svolto il 27 e 28 giugno 2019. Il tema che è stato scelto ha riguardato la trattazione degli aspetti legati al ruolo della cinetica delle reazioni nella modellistica dei fenomeni di interesse in astrofisica, astrochimica, astrobiologia, in occasione della ricorrenza sia dei 160 anni della nascita di Svante Arrhenius, sia dei 130 anni dalla formulazione della sua celebre equazione sulla dipendenza dalla temperatura delle velocità di reazione: i problemi aperti sulle sue basi sperimentali e teorici, la rassegna delle sempre più numerose applicazioni alla modellistica dei processi e le prospettive di sviluppi futuri sono stati posti al centro dell'attenzione.

Parole chiave: Reazioni Chimiche; Teoria ed Esperimenti; Cinetica e Meccanica Statistica; Modelli per Astrochimica, Astrofisica, Astrobiologia

Introduction

The papers collected in this special issue inaugurate the new series of these Memorie: they are contributions that have been prepared on the occasion of an International Conference that was held at the Library of the Italian Academy of Sciences, known as of the Forty, in the Scuderie Vecchie at the prestigious Villa Torlonia in Rome. The meeting follows a series of periodic events hosted by the Academy and organized as an activity of the Study Center dedicated to astrophysics and astrochemistry: it took place on 27 and 28 June 2019. The preceeding Article by President Annibale Mottana is an introduction to the new series of this Journal, which is an essential part of the mission of the Accademia.

Fig. 1 shows the cover of the book extracted from last year's Rendiconti: it contains the collections of the articles originated from the March 2018 event, held on the same venue and sharing the same aim, that of providing a forum for researches interested on the role of molecules in connection with the modern science of the Universe. The book contains a sketch of the history of this discipline, emphasizing the roles of two eminent Academicians, Angelo Secchi in the Nineteenth Century and Gian Gualberto Volpi in the Twentieth. Events are periodically devoted to the first, and the Center for Astrophysics (operating for a few years) is named after the second. The topic characterizing the 2018 event was Molecular Chirality, pervasive in pure and applied chemistry, transversal across several disciplines with relevance also for evolutionary sciences.

The theme that was chosen this year concerned the discussion of aspects related to the role of reaction kinetics in the modelling of phenomena of interest in astrophysics, astrochemistry, astrobiology, on the occasion of both the 160th anniversary of the birth of Svante Arrhenius, and the 130th anniversary of the formulation of his famous equation on the temperature dependence of reaction rates: the open problems on its experimental and theoretical bases, the review of the increasingly numerous applications to process modelling and the prospects for future developments have been placed at the center of the attention of speakers and participants to the lively discussion. Next an account is given of the scientific motivations of the Conference and of this publication. Details and additional information complete this introductory paper.

Astrochemical kinetics

The logo of the Conference is reproduced in Fig. 2. The title emphasizes the role of chemical kinetics for Astrochemistry, a highly interdisciplinary emergent research area, which relies on Earth-based diffuse "observatories" on nature, structure and transformations of the molecular Universe: an inexorably increase of such a multitude of molecules and molecular processes, that couldn't even be imagined only a few decades ago, is detected from spectroscopic and radio-astronomical observations, space-mission data collections, laboratory

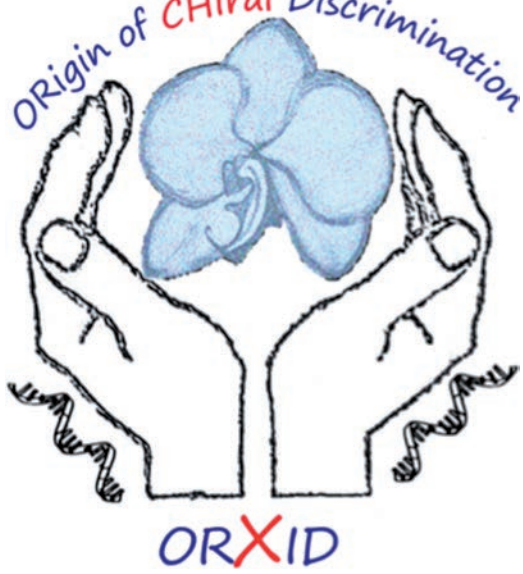

Fig. 1. The cover of the book originated from the 2018 event.

Fig. 2. The logo of the 2019 event, OAK (Art work by Concetta Caglioti).

experiments, computational modelling; they are continuously increasing in number, leading to decisive progress into the understanding of the chemical evolution from the early formation of atomic, molecular, radical, ionic species.

The stepping stones require consolidation by concerted chemical kinetics and molecular dynamics: the meeting aims at connecting experimental and theoretical knowledge by (i) coordinating groups of spectroscopists, astrophysicists, quantum chemists to interact with chemical kineticists within the decade-old established network "Astrochemical Observatory"; (ii) indicating molecular-beam experiments to characterize dynamical and kinetic properties involving interstellar molecules; (iii) assessing role of molecular orientation in chiral discrimination processes, arguably occurring in primordial environments; (iv) developing theoretical models for reactive processes – important those involved in chirality-selective processes and in low-temperature manifestations of non-Arrhenius behavior.

Enrichment of current reaction-rate databases is crucial; tessellation of an immensely wide mosaic, with few sparse pieces known, opens mankind to an arguably infinite search: indeed, there is no certainty that these experimental measurements and theoretical approaches will provide the photodynamic or collisional mechanisms that, for example, played a role in a prebiotic context for the natural emergency of selective chirality: yet, it is an educated guess that they will lead to progress, extending instrumentation and simulation techniques of molecular science in a joint effort of Italian groups with teams already called to collaborate.

An Additional Event and Perspectives

A related twin event preceeded this one in the same week in Rome allowing sharing participants interested in a related multitude of topics. Organizers were Vincenzo Aquilanti, Sergio Carrà, Tommaso Ruggeri. It took place in the premises of the Accademia Nazionale dei Lincei, Palazzo Corsini, Rome on 25-26 June 2019 The title was *Statistical Thermodynamics and Chemical Kinetics: Far Away from Equilibrium*. Basic to the development of modern physical chemistry and of the science of materials, statistical mechanics provides tools for understanding and exploiting the connection between systems at the molecular and macroscopic levels. A topical collection of papers originated from this Conference is currently appearing in the Journal *Rendiconti Lincei, Scienze Fisiche e Naturali*. Purposes and Abstracts are available at the Lincei website. The two events were jointly presented as constituting the Lincei and XL Roman Days of Kinetic Theory and of Chemical Kinetics (June 25-28, 2018). The organizational support by the staff of the National Academy of Sciences, known as of the Forty, and of members of the Department of Excellence for Chemistry, Biology and Biotechnology of the University of Perugia are gratefully acknowledged.

The success of these initiatives and hopefully of these publications are models for us for similar initiatives that had been planned for the year 2020. The Sars Covid 19 pandemia has frustrated our efforts but research in the field has been going on, in spite of unfavorable circumstances, so that when the possibility will arise we are planning to re-establishing a continuity unfortunately interrupted.