



Charles University

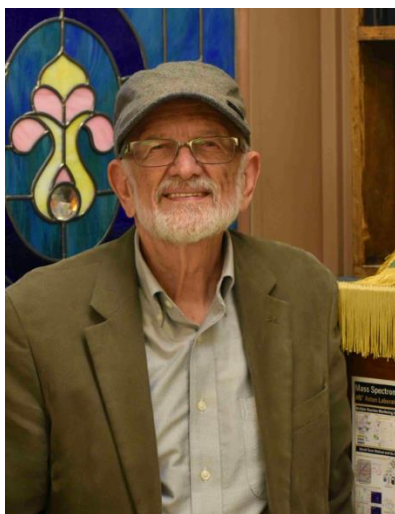
Faculty of Science

Department of Biochemistry



Invites you to attend the lecture:

ACCELERATION OF CHEMICAL REACTIONS IN MICRODROPLETS: PHYSICAL BASIS, HIGH THROUGHPUT ANALYSIS AND IMPLICATIONS FOR DRUG DISCOVERY

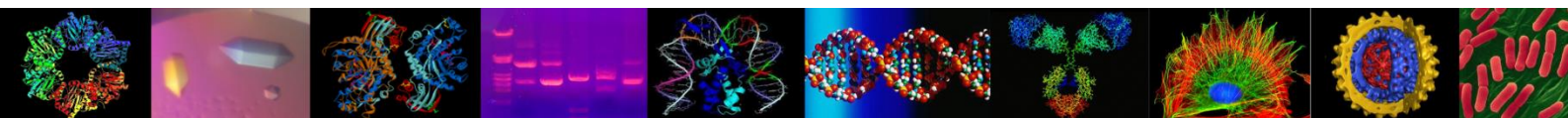


Prof. R. Graham Cooks, PhD.

(Henry Bohn Hass Distinguished Professor of Chemistry
Purdue University, Indiana, USA)

On Tuesday May 9th, 2023 at 10am

Lecture Hall CH2, Chemistry building, Faculty of Science, Hlavova 2030/8, Prague 2



Annotation

This talk introduces the phenomenon of accelerated chemical reactions in microdroplets (rate constants increased by up to a million-fold relative to bulk). The role of the interface will be demonstrated and the general nature of the process in bimolecular processes shown. The underlying factors include partial solvation and high interfacial electric fields. Acceleration occurs in organic as well as aqueous microdroplets. Emphasis is placed on the super-acid and super-base species at interfaces that drive these reactions. Most important is the role of the water radical cation H_2O^+ . And its monohydrate ($\text{H}_2\text{O}^+ \cdot \text{H}_2\text{O}$, especially the isomer $\text{HO} \cdots \text{HO}_2^+$). Redox chemistry of sulfones, phosphonates and ketones will feature. Accelerated reactions occur in desorption electrospray ionization (DESI) mass spectrometry and this allows high throughput (HT) reaction screening (analysis of 6,144 reaction mixtures per hour, at the 5 ng scale). This new capability can be used in small scale synthesis and HT bioassays as the basis for a new approach to the key steps in the drug discovery process.

1. Xin Yan, Ryan M. Bain, and R. Graham Cooks (2016) "Organic Reactions in Microdroplets: Reaction Acceleration Revealed by Mass Spectrometry" *Angew. Chem. Int. Ed.* 55 12960-12972 DOI 10.1002/anie.201602270
2. L. Qiu, R. G. Cooks (2022) Simultaneous and Spontaneous Oxidation and Reduction in Microdroplets by the Water Radical Cation/Anion Pair. *Angew. Chem. Int. Ed.* 61, e2022107; *Angew. Chem.* 134, e2022107.
3. L. Qiu, Z. Wei, H. Nie, R. G. Cooks (2021) Reaction Acceleration Promoted by Partial Solvation at the Gas/Solution Interface. *Chempluschem*, 86, 1362–1365.
4. R. G. Cooks, Y. Feng, K.-H. Huang, N. M. Morato, and L. Qiu (2023) Re-imagining Drug Discovery using Mass Spectrometry. *Isr. J. Chem.* e202300034

Curriculum Vitae

R. Graham Cooks Distinguished Professor at Purdue University and Fellow, National Academy of Sciences and National Academy of Inventors, is a recipient of the Dreyfus Prize. He has served as major professor to 150 PhD students. Research interests include 1) ambient ionization and tandem mass spectrometry analysis of complex mixtures, 2) mass spectrometry in cancer diagnostics and 3) high-throughput synthesis and analysis techniques. Prof. Cooks has published over 1500 research articles, ranks among the most cited chemists worldwide. Several startup companies have emerged from his laboratory.