

ABSTRACT SYMPOSIUM NAME: Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces (Oral)

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: COMP

CONTROL ID: 2992447

PRESENTATION TYPE: Oral Only : Do not consider for Sci-Mix

TITLE: Electron-initiated photochemistry: Molecular ionization, excitation, and reactions

AUTHORS (FIRST NAME, LAST NAME): Karl K. Irikura¹

INSTITUTIONS (ALL):

1. Chemical Sciences Div., National Institute of Standards and Technology, Gaithersburg, MD, United States.

ABSTRACT BODY:

Abstract: Photochemistry is excited-state chemistry where the excited state is prepared by absorbing a photon. Another way to prepare an excited state is impact by a particle. In solution, an incident electron is more likely to strike a solvent molecule than any dilute solute. This is classical pulse radiolysis, in which reactive species are created by destroying solvent molecules. In the gas phase, electron impact on molecules may result in attachment (negative ion), ejection of a secondary electron (ionization), or excitation. Each of these possibilities can lead to chemical reactions, which is what makes plasma chemistry complex and technologically useful. Besides plasma chemistry, another application is electron-ionization mass spectrometry. Mass spectrometry is one of the basic tools of analytical chemistry, yet has evaded a useful theoretical description. This contrasts with photon spectroscopies, for which useful theoretical predictions are routine. I will give an overview of the molecular processes involved in electron-ionization mass spectrometry, making connections with photochemistry. I will also provide one or two examples of catalysis from the broader field of gas-phase ion chemistry.

(No Image Selected)