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Synergistic Study of Hydrocarbon Photochemistry in the Laboratory and Planetary Atmospheres

M. C. Liang (1,2), D. Henze (3), M. Adamkovics (4), E. F. Chu (5), K. Boering (6), and Y. L. Yung (7)

(1) Academia Sinica, Research Center for Environmental Changes, Taipei, Taiwan (mcl@rcec.sinica.edu.tw), (2) Graduate Institute of Astronomy, National Central University, Jhongli, Taiwan, (3) NASA Goddard Institute for Space Studies and the Earth Institute, Columbia University, New York, New York, USA, (4) Department of Astronomy, University of California at Berkeley, Berkeley, USA, (5) Departments of Chemistry and of Earth and Planetary Science, University of California, Berkeley, USA, (6) Department of Chemistry, University of California at Berkeley, Berkeley, USA, (7) Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, USA

A synergistic study of hydrocarbon photochemistry in the laboratory and planetary atmospheres has been carried out using the Caltech/JPL KINETICS photochemical model and laboratory measurements from Adamkovics and Boering (2003). The laboratory simulations provide the data for the time-evolution of gaseous species such as H_2, C_2H_2, C_2H_4, C_2H_6, C_3H_4, C_4H_2 and C_4H_{10} during UV irradiation of CH_4. We apply forward and adjoint models to analyze the experiments. Different photochemical schemes (e.g., Moses et al. 2000, 2005) are compared and modified to reproduce the laboratory results. We first test the full sensitivity of the model results to *all* chemical kinetics using the adjoint model and show that the abundances of C_2H_2, C_2H_4, C_2H_6, and C_4H_{10} can be well reproduced while that of C_4H_2 is underestimated by 1-2 orders of magnitude. The abundance of C_3H_4 is underestimated with Moses et al. (2000) kinetics but overestimated with Moses et al. (2005) kinetics. This suggests a major gap in our understanding of chemical pathways to higher hydrocarbons. We next examine higher order hydrocarbon chemistry ($>C_2$). In this case, we assume that all rate coefficients for the chemistry of C_1 and C_2 hydrocarbons remain invariant in the adjoint optimization. Better agreement is achieved, but complete agreement remains elusive. Further laboratory measurements are urgently needed to constrain the pathways. The implications for modeling the atmospheres of Titan and the giant planets (e.g., Jupiter) are discussed.