Single Pulse Shock Tube Studies on Fundamental Chemical Kinetics, Atmospheric Chemistry, Combustion and Astrophysics/Astrochemistry

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Abstract:
Single pulse shock tube facilities were built in collaboration with the Divisions of Chemical and Mechanical Sciences at the Indian Institute of Science (Figure 1). This can help in raising the T (1000s of K) and P (10 – 100 bar) of a gaseous molecule at a rate of million degrees per second. Our original objectives were to measure activation energies and deduce the mechanism of thermal decomposition of haloalkanes. In particular, chemical activation and thermal activation (carried out in a furnace) studies on 1,2-dichloroethane pyrolysis gave results that were inconsistent appearing to violate transition state/RRKM theories of chemical reactions. Our experiments using the home-made single pulse shock tube resolved this.[1] This facility was used to study the pyrolysis of 2-fluoroethanol, which is a suggested replacement for chlorofluorcarbons which affect the ozone layer.[2] Ignition delays of potential and in-use rocket fuels could be measured and this is an important parameter for the choice of fuels in space/defence applications.[3] Recently, pyrolysis of propargy alcohol was investigated.[4] The first step in this reaction leads to the production of propargyl and hydroxyl radicals, both of which are important in combustion and surprisingly there have been no prior measurements on this important reaction. Propargyl radical is also important in astrophysics as it can dimerize to produce benzene, which eventually leads to soot/dust particles via polycyclic aromatic hydrocarbon in a diesel engine/interstellar space. This facility has been used recently to study the reaction of C + H_2 in order to shed light on how hydrocarbons were formed after big bang.[5] This talk will highlight our journey with shock tubes over the last two decades.

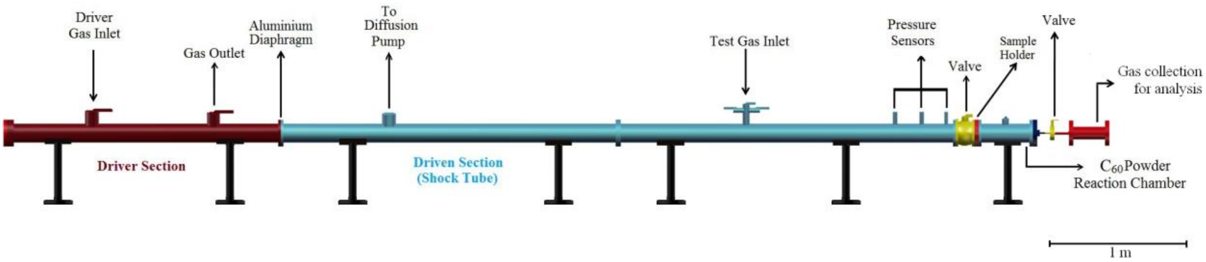

Figure 1. Schematic diagram of a recent version of a single pulse shock tube used for C_{60} + H_2 reaction at high temperature and pressure

References and Notes:

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Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

Bio-Sketch of Speaker

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E. Arunan did his B. Sc. In Chemistry at the American College, Madurai, M.Sc. at the Indian Institute of Technology, Madras and an M. Tech from the Indian Institute of Technology, Delhi. He got his Ph. D. in 1991 under the guidance of Prof. Donald W. Setser at Kansas State University and explored chemical reaction dynamics using infrared chemiluminescence. During his postdoctoral work at the University of Illinois at Urbana-Champaign with Prof. Herbert S. Gutowsky, he used a molecular beam microwave spectrometer and solved longstanding problems including the observation of the fully resolved microwave spectrum of the T-shaped benzene dimer. He then returned back to India to join the Indian Institute of Technology, Kanpur as an Assistant Professor in November 1994 and moved to the Indian Institute of Science in June 1997, where he is currently a Professor at the Department of Inorganic and Physical Chemistry. He has established two experimental laboratories having a molecular beam microwave spectrometer and single pulse shock tubes. His group carried out fundamental work on complexes containing H_2O and H_2S which eventually led to an IUPAC project to redefine hydrogen bonding by a task group formed and chaired by him. IUPAC accepted the recommendation from this task group in 2011. His group was the first to propose a ‘carbon bond’ analogous to a hydrogen bond in 2013 and it has been observed in many chemical and biological systems since then. With shock tube facilities, his group has carried out both fundamental and applied research.

Prof. Arunan is a Fellow of Indian Academy of Sciences and National Academy of Sciences in India, Royal Society of Chemistry and IUPAC. He is an Editor for the Journal of Molecular Structure and a Section-Editor (Chemistry) for Current Science. He was a guest editor for the Annual Reviews in Physical Chemistry, 2016. He is a member of the International Advisory Board for several symposia including the Horizons in Hydrogen Bond Research Conference, International Symposium on Shock Waves, Asian Spectroscopy Conference and is a founder member of a core-group running the annual Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters in India. He is a member of the American Chemical Society, Royal Society of Chemistry and the Chemical Research Society of India. He is also a founding member and Vice-President of the Society for Shock Wave Research in India.