9TH EUROPEAN COMBUSTION MEETING 2019

14 - 17 April, 2019 | Lisboa | Portugal

BOOK OF ABSTRACTS

EDITED BY:
Sandrina Pereira and Mário Costa

Abstract_S3_AII_15

Determination of the rate parameters of N/H/O elementary reactions based on $H_2/O_2/NO_x$ combustion experiments

M. Kovács, T. Varga, C. Olm, Á. Busai, R. Pálvölgyi, I. Gy. Zsély, T. Turányi*
Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary
*turanyi@chem.elte.hu

Abstract
A mechanism for the description of the $H_2/O_2/NO_x$ combustion systems was optimized via the method developed in our laboratory using computer framework code *Optima++*. In total, 5073 experimental data points (ignition delay times, concentration profiles and burning velocity measurements) were collected from the literature and were reproduced using 17 recent NO_x mechanisms. The performance of the Glarborg-2018 mechanism was the best. Ten elementary reactions were selected based on local sensitivity analysis and the Arrhenius parameters of them were fitted to indirect experimental data, and direct experimental and theoretical determinations of the rate coefficients. This way more accurate rate parameters of these reactions were obtained and the temperature dependent uncertainties of the rate coefficients were calculated.