Evaluation of ethyl iodide decomposition shock tube measurements

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Thermal decomposition measurements of ethyl iodide were investigated by kinetic analysis and parameter optimization. The measurements were carried out in shock tube at the Karlsruhe Institute of Technology by Tobias Bentz and Matthias Olzmann [1], [2]. The results of 30 shock tube experiments were investigated, which were carried out in the temperature range of 957–1397 K and pressure range of 1.3–1.8 bar. The time history of H atom concentration was measured using the H-ARAS method. The experimental data were interpreted using a 17-step mechanism, suggested by Tobias Bentz [1]. Local sensitivity analysis was carried out at the conditions of the experiments and it indicated that the rate parameters of the following reactions exhibit high sensitivity at most of the experimental conditions: R1: C_2H_5+M=>C_2H_4+H+M; R2: H+HI=>H_2+I; R4: C_2H_5I=>C_2H_5+I; R5: C_2H_5I=>C_2H_4+HI; R17: C_2H_5I+H=>C_2H_5+HI.
Arrhenius parameters *A* and *E* of these reactions were fitted using the software and computation method described in our recent articles [3], [4]. After the parameter optimization, the simulated H atom curves well coincided with the experimental data. The calculations provided not only the mean values of the fitted parameters, but also their joint covariance matrix. This covariance matrix showed that the rate parameters of reaction R2 can be determined very accurately, and the rate parameters of reactions R1, R5 and R17 can be determined with higher, but acceptable uncertainty. The experimental data do not carry information for the accurate determination of the rate parameters of reaction R4.

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