

Interim report about the activity of IUPAC Task Group No. 2014-028-2-100:
“Chemical kinetics of gas-phase elementary reactions at high temperature”
Period of 1 July, 2018 – 30 June, 2019

The proposal for the creation of the task group was approved on 6 March, 2015. The project leader is Tamás Turányi (ELTE, Budapest). The members of the group are identical to those of the original proposal:

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The discussions within the group were carried out in e-mails. No joint group meeting was held, but during this period the project leader met most of the members of the group in various conferences and meetings, and discussed with them the progress of the tasks.

Preliminary versions of the evaluations have been prepared for the following high-temperature gas-phase elementary reactions:

CH+C₂H₂=products
CH+CH₄=products
CH+H₂O=products
CH+O₂=products
NCN+NO=products
NCN+O₂=products
NCN=C+N₂
CH₂O+H=HCO+H₂
CH₂O+OH=HCO+H₂O
CH₂O+O₂=HCO+HO₂
CH₃O+M=CH₂O+H+M low pressure limit
CH₃OH+H=products
CH₃OH+OH=products

Data sheets in an agreed format were prepared for the reactions above and circulated among the group members.

Dr. Don Burgess in collaboration with a programmer at NIST started to set up a Web site for helping the evaluation of chemical kinetics parameters of gas-phase elementary reactions. This site will help the development of evaluation sheets and promote the discussions within the group as a closed web site. Having reached a consensus for a given elementary reaction,

the content will be opened up to serve the dissemination of the results. In this form it will be one of the NIST online databases. Screen shots of the pages of the web site in its present form have been circulated among the group members for making comments and collecting suggestions. The web site will be online soon, first as an internal web site for the group.

Budapest, 1 July, 2019

Tamás Turányi
Chair of the Task Group