

# Elementary Kinetics Discussion Summary

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- A number of topics were discussed extensively. The main points are summarized on the following slides and some principle points are given below. Interestingly, the group independently arrived at many conclusions similar to those of the Reaction Mechanism discussion group.
- A primary topic of discussion concerned making experimental and theoretical data available in a format that would enable future reevaluation.
- A secondary topic of some concern was the long term status of the NIST kinetics database. All participants in the discussion acknowledged the importance of this database to their research and it is clearly a significant tool for the kinetics research community.
- Concern was expressed, during presentation of the discussion groups findings, that there is only a very limited and shrinking number of people measuring elementary rate coefficients at flame temperatures.

- Sharing Data
  - Common structure for reporting data
    - XML type?
  - Infrastructure
    - PRIME type?
    - More use of supplementary information in journals
      - Attach XML files
      - ASCII files of data

- NIST Kinetics database
  - What is the current status?
  - What will be the long term availability?
  - Can the Combustion community provide support?
  - Can it made more open to help keep it up to date?
    - Upload your data
    - Feedback forms
    - Wikipedia type approach?

- Areas of need for flame chemistry
  - Low temperature chemistry
  - HO<sub>2</sub> reactions
    - Experiment
    - Theory
  - R + O<sub>2</sub>
    - Experimental measurements

- Core reaction mechanism
  - C0, C1, C2....
  - Can a definitive set be established?
  - Is a single core mechanism desirable?
  - How would it be maintained and updated?