Critical Evaluation of Chemical Reaction Rates and Collision Cross Sections of Importance in the Earth's Upper Atmosphere and the Atmospheres of other Planets, Moons, and Comets

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Abstract

We recommend establishment of a long-term program of critical evaluation by domain experts of the rates and cross sections of atomic and molecular processes that are needed for understanding and modeling the atmospheres in the solar system. We envision products resembling those from the ongoing JPL/NASA Panel for Data Evaluation and the efforts of the international combustion modeling community funded by US DOE and its European counterpart. Both of these endeavors already provide some important inputs for modeling the atmospheres of the Earth, planets, moons, and comets. However, their applications restrict the choice of which processes to evaluate and the temperature and pressure ranges to cover, thus leaving large gaps that need to be filled. Interestingly, an older evaluation program once filled some of these gaps. Funded by the US DoD in the 1960s-1980s, the DNA Reaction Rate Handbook provided a thorough treatment of numerous types of collisions and reactions that are important in the Earth's lower ionosphere, and the program even provided funding for new laboratory measurements. Other examples could be given, with the on-line resources at NIST being among the best, but most provide a narrower scope or less critical evaluation. What is needed is not a just a list of processes and numbers (i.e., a "database"), but rather serious comparison of the available information and specific statements from independent expert laboratory/theory data providers about what should be believed, what uncertainty to assign, and what is most in need of redetermination. The major topic areas would include the following: 1. Chemical reactions of neutral atoms and molecules in their ground electronic states 2. Ion-molecule reactions 3. Chemistry, relaxation, and radiation of electronically excited atoms and molecules 4. Vibrational and rotational relaxation and radiation 5. Photoabsorption, photodissociation, and photoionization 6. Electron-impact excitation, dissociation,

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ionization, and recombination 7. Energetic heavy particle excitation and charge exchange