High Level Ab Initio Kinetics as a Tool for Astrochemistry

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Résumé

We will survey the application of ab initio theoretical kinetics to reactions of importance to astrochemistry. Illustrative examples will be taken from our calculations for (i) interstellar chemistry, (ii) Titan's atmospheric chemistry, and (iii) the chemistry of extrasolar giant planets. The accuracy of various aspects of the calculations will be summarized including (i) the underlying ab initio electronic structure calculations, (ii) the treatment of the high pressure recombination process, and (iii) the treatment of the pressure dependence of the kinetics. The applications will consider the chemistry of phosphorous on giant planets, the kinetics of water dimerization, the chemistry of nitrogen on Titan's atmosphere, as well as various reactions of interstellar chemistry interest such as the recombination of OH with H, and O(3P) reacting with C2H5, CH2, and CCS.

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