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Prebiotic Atmospheric Chemistry on Titan: Formation Kinetics via Ab Initio Calculations for Potential Energy Surface (PES) Mapping
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— It has been recently shown that Titan provides a unique perspective in our solar system: its atmosphere is comparable to a model of prebiotic Earth's. Provided the organic cationic and anionic molecular species identified by the Cassini spacecraft, this research characterizes reaction pathways for the reactions of methyl derivatives of the cyclopropenyl cation, the methyl cation with methyl- and dimethyl-acetylene, and reactions of resonance structures of protonated acrylonitrile with CH2NH. Isomerization and dissociation reactions involving methyl-cyclopropenyl cations, the perinaphthenyl cation and anion, and cations of pyrimidine and purine precursors of nucleobases will be examined to locate reaction pathways, intermediates, transition states, and products of the reactions. Gaussian '09 software is used for ab initio calculations to map out the PES. Geometry optimizations and vibrational frequency computations are preformed via the double-hybrid density functional B2PLYP-D3. Single-point energies are refined by use of the explicitly-correlated coupled-cluster CCSD(T)-F12 method. Rate constants are calculated using microcanonical RRKM theory, and pressure effects evaluated used the Master Equation approach; these allow for prediction of absolute rate constants and product branching ratios at different pressures and temperatures.

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