MODELING OF SIMPLE AROMATIC SPECIES UNDER DARK CLOUD CONDITIONS

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The very recent discoveries of monocyclic and bicyclic aromatic molecules in rotational emission suggest that small aromatic molecules may actively form in prestellar dark clouds (McGuire et al. 2018, 2021). Although the high densities ($\sim 10^4$ cm^{-3}) allow molecules in dark clouds to collide and stick to grains and the low temperature ($\leq$10 K) further precludes thermal evaporation (Bergen 2003), benzonitrile, a monocyclic aromatic molecule, is still observed toward multiple prestellar environments (Burkhardt et al. 2021). In this talk, we will present our efforts to numerically model these simple aromatic molecules with the rate-equation-based kinetic code, Nautilus, in dark cloud environments. To produce a more comprehensive chemical network for aromatics, we systematically added new species that may serve as precursors to the aromatic species and pathways leading to the formation of the most fundamental aromatic species, benzene (C_6H_6), under low temperature and high density conditions. In particular, we examined possible formation pathways, including the ion-molecule reaction of ethynyl radical (CCH) and 1,3-butadiene ($CH_2CHCHCH_2$), the neutral-neutral reaction of acetylene (HCCH) and vinyl acetylene (CH_2CHC_2H), and the dissociative recombination reaction of benzenium ions ($C_6H_7^+$). Although the current model under-predicts the observed abundance of both monocyclic and bicyclic aromatic molecule, the updates we have made to the reaction network of related species have shown substantial progress in bringing the models into alignment with observations. Our results suggest that viable reactions forming and releasing small aromatic molecules on grains may be necessary to bridge the gap between models and observations in prestellar dark clouds.