MODELING SOME NEWLY DETECTED MOLECULES

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Seven interstellar molecules have been recently detected for the first time or confirmed via their rotational spectra with the Green Bank Telescope (GBT). Towards the cold interstellar core TMC-1, two isomers of C_4H_3N, cyanoallene (CH_2CCHCN) and methylcyanoacetylene (CH_3CCCN), as well as methyl-cyano-diacetylene (CH_3C_5N), and methyl-triacetylene (CH_3C_6H) were found. Towards the complex galactic center source Sgr B2, cyclopropenal (c-C_3H_2O) , ketenimine (CH_2CNH), and acetamide (CH_3CONH_2) were observed. Here we report a detailed study of the chemistry underlying possible formation pathways of these molecules. Starting with our updated gas-phase chemical reaction network osu.2007 (see http://www.physics.ohio-state.edu/ eric/), we added many possible reactions involving the formation and depletion of each observed molecule, and simulated the gas-phase chemistry as a function of time for both sources. For TMC-1, we reproduced the observed fractional abundances of all four detected molecules at typical times of 10^{5-6} yr . For the complex star-forming region Sgr B2, our gas-phase simulation was less successful. It is reasonably clear that surface chemistry followed by desorption into the gas plays an important role in the portions of Sgr B2 studied with the GBT.