GAS-GRAIN MODELING OF HNCO, HOCN, HCNO, AND HONC

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Among isomers made of H, C, N, and O, the lowest energy isomer, isocyanic acid (HNCO), has been detected towards various interstellar sources, ranging from cold dense cores such as TMC-1 to hot cores such as SgrB2(M). One metastable isomer, fulminic acid (HCNO), has been detected in cold cores, as well as the lukewarm core L1527 (Marcelino et al., 2009, ApJ 690, L27). Here we present gas-grain model studies of HNCO and HCNO, as well as two other isomers, cyanic acid (HOCN) and isofulminic acid (HONC). We apply four models: a warm-up hot core model where T starts at 10 K and increases to 200 K over a time of 2×10^5 yr and then remains at 200 K; a warm-up hot-core envelope model where T increases from 10 K to 50 K over the same time period; a warm-up lukewarm model where T increases from 10 K to 30 K; and a model where T remains constant at 10 K. In the hot core warm-up model, the increase in temperature produces an increase in gas-phase abundance for all four isomers. In the envelope warm-up model, the HNCO and HOCN abundances increase, the HCNO abundance is unchanged, while HONC slightly decreases as T increases. In the lukewarm model, within the time range investigated, both calculated HNCO and HCNO fractional abundance in the gas phase are in good agreement with observed abundances except at the very beginning. HOCN shows a low calculated abundance before 1×10^4 yr, after which it starts increasing and reaches relatively detectable value of 7×10^{-11} and remains abundant afterwards. In the constant low temperature model, the observed fractional abundance of HNCO towards TMC-1 is reproduced at a time of $\approx 1 \times 10^5$ yr, at which time the other two isomers have abundances about two orders of magnitude lower than HNCO, a result in reasonable agreement with the gas-phase steady-state model of Marcelino et al.