

Interstellar HNCO, HOCN and HCNO: gas-grain modeling approach.

DONGHUI QUAN, *Chemical Physics Program, The Ohio State University, Columbus, OH 43210*;
ERIC HERBST, *Departments of Physics, Astronomy, & Chemistry, The Ohio State University,
Columbus, OH 43210*.

HNCO is a well-known interstellar molecule, which has been detected towards various sources. Recently two of its isomers, HOCN and HCNO, were newly detected: HOCN was detected towards the hot core source Sgr B2(M), while HCNO was detected in several cold cores. Here we present three gas-grain model studies of all these three molecules: a warm-up hot core model where T starts from 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; 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 three isomers. At their peak abundances (200 K), HOCN and HNCO are predicted to lie well above their observed values towards Sgr B2(M). In the envelope warm-up model, the HNCO and HOCN abundances increase while the HCNO abundance is unchanged as T increases. Here both HOCN and HNCO have peak abundances (50 K) in reasonable agreement with the observed abundances towards Sgr B2(M). 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 models.