

VARIABLE-TEMPERATURE  $^1\text{H}$ -NMR AND AB INITIO STUDY OF 5-  
AMINO-IMIDAZOLE-4-CARBOXAMIDE (AICA):  
COMPETING PATHS FOR AMIDE-H SCRAMBLING

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ABSTRACT

5(4)-aminoimidazole-4(5)-carboxamide (AICA and TAICA) is an important precursor for the synthesis of purines in general and of the nucleobases adenine and guanine in particular. Biotic nucleobase synthesis has been studied in great detail and its chemistry and biochemistry are understood very well. In contrast, hypotheses regarding prebiotic nucleobase syntheses remain controversial. While such studies focused on aqueous solution chemistry for half a century, planetary nucleobase syntheses in frozen solids (ice) and other extreme environments have been explored in the past two decades. Spectacular advances in observational astronomy and the evolving knowledge about the chemistry and physics of the interstellar medium (ISM) suggest new options and the very possibility of prebiotic nucleobase synthesis in the cold ISM.

The discourse about prebiotic chemistry in interstellar space relies on observational astronomy. Hence, precise knowledge is required about the spectroscopic properties of presumed intermediates together with knowledge of their structural preferences and their isomerization dynamics. Here, we report on the structure and dynamics of AICA in a variety of solvents and the gas phase. The interplay between CC- and CN- rotations are discussed as well.