

PRODUCTION OF HOCH₂CO, HOCHCHO, AND HOCHCO IN THE REACTION H + GLYCOLALDEHYDE (HOCH₂CHO) IN SOLID *p*-H₂ AND ITS IMPLICATION IN ASTROCHEMISTRY

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Glycolaldehyde (HOCH₂CHO) has been detected in the interstellar medium; it is considered to play an important role in the formation of complex organic molecules, especially higher sugars. We took the advantages of unique properties of *para*-hydrogen (*p*-H₂), which serves as a quantum-solid matrix host and a medium for efficient hydrogen-atom reaction, to investigate the reaction between HOCH₂CHO and H atoms. H atoms were generated on photolysis at 365 nm of a co-deposited mixture of HOCH₂CHO/*p*-H₂ and Cl₂ and subsequent IR irradiation for promoting the Cl + H₂ ($\nu = 1$) → H + HCl reaction. Based on the orientation of O-H and C=O bonds, HOCH₂CHO has 4 conformers; *cis-cis* conformer is found to have the least energy among all due to the intramolecular H-bonding. In the reaction H + HOCH₂CHO at 3.2 K, 5 lines in the first group and 6 lines in the second group are assigned to HOCH₂CO and HOCHCHO radicals, products of the first H-abstraction from -CHO and -CH₂ groups, respectively. In addition, 2 lines were assigned to HOCHCO, a product of the second H-abstraction. IR irradiation employed during H-atoms generation was also responsible for the conformational conversion of HOCH₂CHO, *cc* → *tt*; which intricates the H + *cc*-HOCH₂CHO reaction to some extent. Since photolysis at 266 nm also promotes this conversion; we photolyzed the *cc*-HOCH₂CHO at 266 nm prior to 365 nm/IR irradiation for complete conversion to the *tt*-form to facilitate the H + *tt*-HOCH₂CHO reaction. Four lines in one group and 3 lines in the second group, those differ from their *cc*-form analogs, were assigned to the *tt*-HOCH₂CO and *tt*-HOCHCHO radicals, respectively; 2 lines in the third group were assigned to HOCHCO. Besides these assignments, a line at 2079.3 cm⁻¹ was tentatively assigned to the OCHCO radical, a product of the third H-abstraction. The assignments of all these products agree satisfactorily with vibrational wavenumbers predicted with the B3LYP/aug-cc-pVTZ method. The PES of H + *cc*- and *tt*-HOCH₂CHO reactions reveal the feasibility of H-abstraction processes for HOCH₂CO, HOCHCHO, HOCHCO, and OCHCO formations after sequential H-abstractions from the CHO, CH₂, CH₂/CHO, and OH moieties, respectively.