

INFRARED SPECTRUM OF THE 1-IODOPROPYL RADICAL PRODUCED FROM REACTION OF I + PROPENE IN SOLID PARA-HYDROGEN

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The addition reactions of iodine atom with propene in solid para-hydrogen (p-H₂) matrices were investigated with infrared (IR) absorption spectroscopy. Mixtures of propene and I₂ seeded in p-H₂ were co-deposited at 3.3 K for 7 to 8 hours, followed by irradiations with ultraviolet lights at various wavelengths to study the reaction of I atoms with propene. Quantum chemical calculations were carried out at the B3LYP/aug-cc-pVTZ-pp level in order to determine the relative energies, vibrational wavenumbers and IR intensities of 1-iodopropyl and 2-iodopropyl radicals. The transitions belong to I₂-propene complex, 1-iodopropyl radical, and the anti conformer of 1,2-diiodopropane were recorded and assigned. The assignments were based on expected reaction, the vibrational wavenumbers and IR intensities from theoretical calculations, and secondary photolysis behavior. The observation of 1-iodopropyl radical, the isomer with the least energy, indicates that the addition of iodine atom occurs at the terminal carbon atom. The role of the p-H₂ matrices, the difference between this reaction and the previously reported Cl + propene reaction will be discussed.