INFRARED SPECTRA OF THE 2-CHLOROETHYL RADICAL IN SOLID PARA-HYDROGEN

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The reaction of chlorine atoms with ethylene and two of its deuterium isotopomers in solid $para$-hydrogen (p-H_2) matrices at 3 K has been studied using infrared spectroscopy. Irradiation at 365 nm of a co-deposited mixture of Cl_2, C_2H_4, and p-H_2 at 3 K produces a series of new lines in the infrared spectrum. Several of the new lines are readily assigned to the gauche and trans conformers of 1,2-dichloroethane (CH_2ClCH_2Cl) resulting from the addition of two Cl atoms to C_2H_4. Of the remaining lines, a strong line at 664 cm^{-1} and three weaker lines at 562, 1070, and 1228 cm^{-1} are concluded to be due to a single carrier based on their behavior upon subsequent annealing to 4.5 K and irradiation at 254 and 214 nm. When the positions and intensities of these lines are compared to the MP2/aug-cc-pVDZ predicted vibrational spectra of the possible species that could result from the addition and abstraction reactions of one Cl atom with C_2H_4[a], the best agreement is found with the 2-chloroethyl radical ($\cdot CH_2CH_2Cl$). In order to confirm this assignment, isotopic experiments were performed with C_2D_4 and t-$C_2H_2D_2$ and the corresponding infrared bands due to the deuterium isotopomers of this radical ($\cdot CD_2CD_2Cl$ and $\cdot CHDCHDCl$) have been observed. A final set of experiments were performed following irradiation of the $Cl_2/C_2H_4/p$-H_2 mixture at 365 nm, in which the matrix was irradiated with filtered infrared light from a globar source, which has been shown to induce a reaction between isolated Cl atoms and matrix H_2 to produce HCl and H atoms[b]. In our experiments, the major products observed were HCl and ethyl chloride (CH_3CH_2Cl) and the possible mechanism of the formation of ethyl chloride will be discussed.

[a] P. Brana, B. Menendez, T. Fernandez, and J. A. Sordo, J. Phys. Chem. A 104, 10842 (2000)
[b] P. L. Raston and D. T. Anderson, Phys. Chem. Chem. Phys. 8, 3124 (2006)