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Nonactivated adsorption of CH_3Cl on Si(100)-2×1 studied by LEED, AES and semiempirical method.

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The adsorption processes of methyl chloride on Si(100)-2×1 have been studied by low energy electron diffraction (LEED), Auger electron spectroscopy (AES) and semiempirical PM3 calculations. The dissociative adsorption of the methyl chloride on Si(100) takes place without breaking of the silicon dimer with high efficiency. For adsorption at the room temperature, the existence of a precursor state is confirmed by the behavior of the sticking probability depending on the coverage and temperature. From AES measurements, the determined activation barrier of adsorption ($\triangle H_{ads}$) is -28.4 kj/mol. This results indicate that the dissociative process is nonactivated. The optimized precursor state of CH_3Cl on the Si(100)-2×1 surface was determined by PM3 calculations based on a cluster model.