Vibrational SFG Spectra of 
n-Octadecyltrichlorosilane Monolayers Chemisorbed on 
SiO$_2$-deposited CaF$_2$ Substrates

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**Introduction.** Infrared (IR)-visible/UV sum-frequency generation (SFG) spectroscopy is a method for measuring vibrational spectra of interface molecules. Because only surface or interface species give a resonant contribution to SFG signal, the technique is highly surface-specific and has been developed into a very powerful surface analytical tool. Aiming to measure SFG spectra of organic monolayers silanized on solid surfaces in aqueous environment, we have developed a new type of substrates that allow silanization and are transparent over a broad range of the IR probe. The silanized monolayers are robust, chemically stable, and can serve to surface-immobilize various types of biological molecules.

**Experimental.** The newly developed substrates comprise a thin SiO$_2$ layer (a few hundreds nanometer scale) overlying a CaF$_2$ (1 mm) plate. n-Octadecyltrichlorosilane (OTS) monolayers were chemisorbed onto pure SiO$_2$ and SiO$_2$/CaF$_2$ substrates under the same silanization condition. Fig. 1 depicts the layouts of the OTS samples on the two types of substrates. The SFG spectra were measured with ppp (SFG, visible, IR)- and ssp-polarization combinations.

**Results and Discussion.** Fig. 2 shows the normalized SFG spectra of the OTS monolayers on the SiO$_2$ and SiO$_2$/CaF$_2$ substrates. The spectral features obtained from the two samples are essentially identical for both polarization modes. Three peaks at 2965, 2940, and 2880 cm$^{-1}$ are dominant, all of which are attributed to the CH stretching ($\nu$(CH)) modes of the terminal methyl groups. Because the $\nu$(CH) bands of the methylene groups in all-*trans* alkyl chains are SFG inactive, these results suggest that the OTS molecules on both types of substrates are oriented in the same all-*trans* conformation, indicating the usability and efficiency of the SiO$_2$-deposited CaF$_2$ substrate.